David C Clary

List of Publications by Year
in descending order

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356 papers	17,259 citations	17440 63 h-index	20961 115 g-index
376 all docs	376 docs citations	376 times ranked	8009 citing authors

#	Article	IF	Citations
1	Computational analyses of the vibrational spectra of fentanyl, carfentanil and remifentanil. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 270, 120763.	3.9	2
2	Amyand David Buckingham. 28 January 1930â€”4 February 2021. Biographical Memoirs of Fellows of the Royal Society, 2022, 72, 77-99.	0.1	0
3	Computational molecular spectroscopy. Nature Reviews Methods Primers, 2021, 1, .	21.2	73
4	Calculations on the unimolecular decomposition of the nerve agent VX. Physical Chemistry Chemical Physics, 2020, 22, 564-574.	2.8	3
5	Hydrogen tunnelling in the rearrangements of carbenes: the role of dynamical calculations. Physical Chemistry Chemical Physics, 2020, 22, 962-965.	2.8	5
6	Analytic Route to Tunneling Splittings Using Semiclassical Perturbation Theory. Journal of Chemical Theory and Computation, 2020, 16, 3486-3493.	5.3	10
7	Tunnelling in cyclocarbenes: An application of Semiclassical Transition State Theory in reduced dimensions. Chemical Physics Letters, 2019, 735, 136783.	2.6	2
8	New Developments in Semiclassical Transition-State Theory. Journal of Physical Chemistry A, 2019, 123, 4639-4657.	2.5	27
9	Theoretical Study of Gas-Phase Unimolecular Decomposition of Simulants of the Nerve Agent VX. Journal of Physical Chemistry A, 2019, 123, 59-72.	2.5	10
10	Application of one-dimensional semiclassical transition state theory to the CH ₃ OH + H â‡Œ CH ₂ OH/CH ₃ O + H ₂ reactions. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2018, 376, 20170147.	3.4	11
11	Modern theoretical chemistry: the legacy of Prof. John N. Murrell. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2018, 376, 20170460.	3.4	0
12	Tunnelling and the kinetic isotope effect in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si114.gif" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CH</mml:mtext></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:r Chemical Physics Letters, 2018, 693, 88-94.	2.6	13
13	Precise characterisation of isolated molecules: general discussion. Faraday Discussions, 2018, 212, 137-155.	3.2	1
14	Quantum dynamics of isolated molecules: general discussion. Faraday Discussions, 2018, 212, 281-306.	3.2	0
15	Molecules in confinement in clusters, quantum solvents and matrices: general discussion. Faraday Discussions, 2018, 212, 569-601.	3.2	4
16	Catalysis and tunnelling in the unimolecular decay of Criegee intermediates. Physical Chemistry Chemical Physics, 2018, 20, 25224-25234.	2.8	12
17	Spiers Memorial Lecture : Introductory lecture: quantum dynamics of chemical reactions. Faraday Discussions, 2018, 212, 9-32.	3.2	7
18	John Norman Murrell. 2 March 1932 â€” 25 January 2016. Biographical Memoirs of Fellows of the Royal Society, 2017, 63, 467-486.	0.1	1

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19	A Combined Theoretical and Experimental Study of Sarin (GB) Decomposition at High Temperatures. Journal of Physical Chemistry A, 2017, 121, 6200-6210.	2.5	24
20	Recent advances in quantum scattering calculations on polyatomic bimolecular reactions. Chemical Society Reviews, 2017, 46, 7625-7649.	38.1	72
21	A Tribute to Ahmed H. Zewail. , 2017, , 47-53.		0
22	Ahmed Zewail (1946â€“2016): Commemoration Issue of Chemical Physics Letters. Chemical Physics Letters, 2017, 683, 1-6.	2.6	1
23	Chemical reaction dynamics. Chemical Society Reviews, 2017, 46, 7481-7482.	38.1	14
24	An investigation of one- versus two-dimensional semiclassical transition state theory for H atom abstraction and exchange reactions. Journal of Chemical Physics, 2016, 144, 084113.	3.0	22
25	Fundamentals: general discussion. Faraday Discussions, 2016, 195, 139-169.	3.2	2
26	Rate constants of chemical reactions from semiclassical transition state theory in full and one dimension. Journal of Chemical Physics, 2016, 144, 244116.	3.0	27
27	Quantum dynamics in the smallest water droplet. Science, 2016, 351, 1267-1268.	12.6	36
28	Reduced-Dimensionality Semiclassical Transition State Theory: Application to Hydrogen Atom Abstraction and Exchange Reactions of Hydrocarbons. Journal of Physical Chemistry A, 2015, 119, 12015-12027.	2.5	21
29	Quantum Dynamics of the Abstraction Reaction of H with Cyclopropane. Journal of Physical Chemistry A, 2014, 118, 10134-10143.	2.5	13
30	Historical perspective on: â€œSemiclassical trajectory approach to photoisomerisationâ€•by A Warshel and M. Karplus [Chem. Phys. Lett. 32 (1) (1975) 11â€“17]. Chemical Physics Letters, 2013, 589, 67.	2.6	0
31	100 Years of Atomic Theory. Science, 2013, 341, 244-245.	12.6	1
32	A reduced dimensionality quantum mechanical study of the H + HCF3 â†” H2 + CF3 reaction. Physical Chemistry Chemical Physics, 2013, 15, 18530.	2.8	8
33	Crossed-beam and reduced dimensionality studies of the state-to-state integral cross sections of the Cl+HCD3(v)â†'HCl(vâ€²)+CD3 reaction. Chemical Physics Letters, 2013, 587, 88-92.	2.6	9
34	Quantum effects in the abstraction reaction by H atoms of primary and secondary hydrogens in n-C4H10: a test of a new potential energy surface construction method. Physical Chemistry Chemical Physics, 2013, 15, 1222-1231.	2.8	16
35	Quasiclassical trajectory calculations of hydrogen absorption in the (NaAlH4)2Ti system on a model analytical potential energy surface. Physical Chemistry Chemical Physics, 2012, 14, 3915.	2.8	2
36	Reactive resonances in the F + CHD3 reactionâ€”a quantum dynamics study. Physical Chemistry Chemical Physics, 2011, 13, 4340.	2.8	25

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37	A multifaceted approach to hydrogen storage. Physical Chemistry Chemical Physics, 2011, 13, 16955.	2.8	64
38	Definition of the hydrogen bond (IUPAC Recommendations 2011). Pure and Applied Chemistry, 2011, 83, 1637-1641.	1.9	1,449
39	Defining the hydrogen bond: An account (IUPAC Technical Report). Pure and Applied Chemistry, 2011, 83, 1619-1636.	1.9	856
40	An efficient route to thermal rate constants in reduced dimensional quantum scattering simulations: Applications to the abstraction of hydrogen from alkanes. Journal of Chemical Physics, 2011, 135, 094311.	3.0	28
41	Reduced dimensionality spin-orbit dynamics of CH3 + HCl $ightleftharpoons$â‡Œ CH4 + Cl on ab initio surfaces. Journal of Chemical Physics, 2011, 134, 204311.	3.0	36
42	Towards understanding a mechanism for reversible hydrogen storage: theoretical study of transition metal catalysed dehydrogenation of sodium alanate. Physical Chemistry Chemical Physics, 2010, 12, 4012.	2.8	20
43	An improved treatment of spectator mode vibrations in reduced dimensional quantum dynamics: Application to the hydrogen abstraction reactions Î¼+CH4, H+CH4, D+CH4, and CH3+CH4. Journal of Chemical Physics, 2009, 131, 044111.	3.0	31
44	Reduced Dimensionality Quantum Dynamics of CH₃ + CH₄ â†' CH₄ + CH₃: Symmetric Hydrogen Exchange on an Ab Initio Potential. Journal of Physical Chemistry A, 2009, 113, 4255-4264.	2.5	26
45	Chemical reaction surface vibrational frequencies evaluated in curvilinear internal coordinates: Application to H+CH4â‡ŒH2+CH3. Journal of Chemical Physics, 2009, 130, 024106.	3.0	25
46	Femtochemistry and femtobiology. Chemical Physics, 2008, 350, 1.	1.9	3
47	Quantum Dynamics of Chemical Reactions. Science, 2008, 321, 789-791.	12.6	53
48	Theoretical studies on bimolecular reaction dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 12649-12653.	7.1	52
49	Quantum study on the branching ratio of the reaction NO2+OH. Journal of Chemical Physics, 2007, 126, 154321.	3.0	10
50	Reduced dimensionality quantum dynamics of Cl + CH4? HCl + CH3 on an ab initio potential. Physical Chemistry Chemical Physics, 2007, 9, 933.	2.8	52
51	Torsional anharmonicity in the conformational analysis of tryptamine. Physical Chemistry Chemical Physics, 2007, 9, 2065.	2.8	15
52	Torsional anharmonicity in transition state theory calculations. Physical Chemistry Chemical Physics, 2007, 9, 2397.	2.8	19
53	Quantum scattering study of the abstraction reactions of H atoms from CH3NH2. Chemical Physics Letters, 2007, 438, 1-7.	2.6	26
54	Quantum dynamics study of the Langmuirâ€"Hinshelwood H+H recombination mechanism and H2 formation on a graphene model surface. Chemical Physics, 2007, 338, 1-10.	1.9	20

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55	Quantum reactive scattering of H + hydrocarbon reactions. Physical Chemistry Chemical Physics, 2006, 8, 917.	2.8	56
56	Comparative study of cluster- and supercell-approaches for investigating heterogeneous catalysis by electronic structure methods: Tunneling in the reaction N + H â† NH on Ru(0001). Physical Chemistry Chemical Physics, 2006, 8, 1437.	2.8	21
57	Predicting Catalysis:Â Understanding Ammonia Synthesis from First-Principles Calculations. Journal of Physical Chemistry B, 2006, 110, 17719-17735.	2.6	192
58	Rates of the reaction C2H3+H2â†'C2H4+H. Molecular Physics, 2006, 104, 151-158.	1.7	7
59	Torsional Anharmonicity in the Conformational Analysis of Î²-d-Galactoseâ€. Journal of Physical Chemistry B, 2006, 110, 3485-3492.	2.6	11
60	Quantum Simulation of a Hydrated Noradrenaline Analog with the Torsional Path Integral Methodâ€. Journal of Physical Chemistry A, 2006, 110, 731-740.	2.5	13
61	Excitement of molecules on surfaces. Nature Materials, 2006, 5, 345-346.	27.5	1
62	Quantum dynamics calculations of the Mu+CH4â†'MuH+CH3 reaction rate constants. Chemical Physics Letters, 2006, 421, 499-503.	2.6	13
63	Rate constant calculations on the N(4S)+OH(2Î) reaction. Chemical Physics Letters, 2006, 431, 261-266.	2.6	33
64	The thermodesorption mechanism of ammonia from Ru(0001). Surface Science, 2006, 600, 1054-1059.	1.9	3
65	Reaction rates of all hydrogenation steps in ammonia synthesis over a Ru(0001) surface. Journal of Catalysis, 2006, 244, 199-207.	6.2	14
66	CHEMISTRY: Quantum Chemistry of Complex Systems. Science, 2006, 314, 265-266.	12.6	19
67	The importance of tunneling in the first hydrogenation step in ammonia synthesis over a Ru(0001) surface. Journal of Chemical Physics, 2005, 122, 134702.	3.0	19
68	The effect of the torsional and stretching vibrations of C2H6 on the H+C2H6â†'H2+C2H5 reaction. Journal of Chemical Physics, 2005, 123, 064305.	3.0	20
69	Collision-induced conformational changes in glycine. Journal of Chemical Physics, 2005, 122, 244323.	3.0	32
70	CHEMISTRY: Geometric Phase in Chemical Reactions. Science, 2005, 309, 1195-1196.	12.6	14
71	Quantum dynamics and kinetics of the abstraction reactions by H atoms of primary and secondary hydrogens in C3H8. Molecular Physics, 2005, 103, 1745-1755.	1.7	16
72	Nuclear quantum effects on the structure and energetics of (H2O)6H+. Physical Chemistry Chemical Physics, 2005, 7, 2324.	2.8	40

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73	Torsional anharmonicity in the conformational thermodynamics of flexible molecules. Molecular Physics, 2005, 103, 1573-1578.	1.7	19
74	Quantum initial value representation simulation of water trimer far infrared absorption spectrum. Journal of Chemical Physics, 2004, 120, 5608-5615.	3.0	18
75	Ab initiorate constants from hyperspherical quantum scattering: Application to H+CH4â†'H2+CH3. Journal of Chemical Physics, 2004, 120, 2308-2318.	3.0	63
76	Ab initiorate constants from hyperspherical quantum scattering: Application to H+C2H6 and H+CH3OH. Journal of Chemical Physics, 2004, 121, 6809-6821.	3.0	49
77	Computational studies of proteinâ€"peptide interactions with systematic mutation of residues. Molecular Physics, 2004, 102, 939-951.	1.7	2
78	Predicting Conformations of Biomolecules:â€‰ Application to a Noradrenaline Analogue. Journal of Physical Chemistry B, 2004, 108, 2484-2488.	2.6	21
79	Theoretical Investigation of the Surface Reaction N(ads)+ H(ads)â†' NH(ads)on Ru(0001) Using Density Functional Calculations, Variational Transition-State Theory, and Semiclassical Tunneling Method. Journal of Physical Chemistry B, 2004, 108, 336-345.	2.6	14
80	Quantum-mechanical calculations on pressure and temperature dependence of three-body recombination reactions: Application to ozone formation rates. Journal of Chemical Physics, 2004, 120, 2700-2707.	3.0	51
81	Kinetic Isotope Effects in the Reactions of D Atoms with CH4, C2H6, and CH3OH: Quantum Dynamics Calculationsâ€. Journal of Physical Chemistry A, 2004, 108, 8966-8972.	2.5	49
82	Quantum free energies of the conformers of glycine on an ab initio potential energy surfaceElectronic supplementary information (ESI) available: Calculated harmonic frequencies of the glycine conformers. See http://www.rsc.org/suppdata/cp/b3/b314644h/. Physical Chemistry Chemical Physics, 2004, 6, 2563.	2.8	55
83	Observational Indicators of Formation Excitation of H2. Astrophysics and Space Science, 2003, 288, 377-389.	1.4	19
84	Vibrational relaxation in H2+H2: full-dimensional quantum dynamical study. International Journal of Mass Spectrometry, 2003, 223-224, 335-342.	1.5	14
85	Surface Coverage Effects on the Formation of Molecular Hydrogen on a Graphite Surface via an Eleyâ^'Rideal Mechanism. Journal of Physical Chemistry A, 2003, 107, 10862-10871.	2.5	20
86	QUANTUMSCATTERINGCALCULATIONS ONCHEMICALREACTIONS. Annual Review of Physical Chemistry, 2003, 54, 493-529.	10.8	371
87	A Simplified Reduced-Dimensionality Study to Treat Reactions of the Type X + CZ3Y â†' XY + CZ3â€. Journal of Physical Chemistry A, 2003, 107, 10851-10856.	2.5	23
88	Zero temperature quantum properties of small protonated water clusters (H2O)nH+ (n=1â€"5). Journal of Chemical Physics, 2003, 119, 10048-10062.	3.0	54
89	Torsional path integral Monte Carlo method for calculating the absolute quantum free energy of large molecules. Journal of Chemical Physics, 2003, 119, 68-76.	3.0	36
90	Microscopic mechanisms for photoinduced metastability in amorphousAs2S3. Physical Review B, 2002, 65, .	3.2	15

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91	Excitation of torsional modes of proteins via collisional energy transfer: A quantum dynamical approach. Journal of Chemical Physics, 2002, 116, 9829-9838.	3.0	25
92	Quantum-mechanical calculations on termolecular association reactions XY+Z+Mâ†'XYZ+M: Application to ozone formation. Journal of Chemical Physics, 2002, 117, 1660-1672.	3.0	61
93	Calculation of the energy levels of weakly bound molecular trimers: Application to (H2)3. Journal of Chemical Physics, 2002, 117, 7512-7519.	3.0	19
94	C + C2H2: A Key Reaction in Interstellar Chemistry. Journal of Physical Chemistry A, 2002, 106, 5541-5552.	2.5	78
95	Isotope Effects in the Formation of Molecular Hydrogen on a Graphite Surface via an Eleyâ^'Rideal Mechanism. Journal of Physical Chemistry A, 2002, 106, 8996-9008.	2.5	28
96	Rate Constants for the CH4 + H â†' CH3 + H2 Reaction Calculated with a Generalized Reduced-Dimensionality Method. Journal of Physical Chemistry A, 2002, 106, 8256-8260.	2.5	44
97	Torsional path integral Monte Carlo method for the quantum simulation of large molecules. Journal of Chemical Physics, 2002, 116, 8262.	3.0	30
98	A full-dimensional quantum dynamical study of vibrational relaxation in H2+H2. Chemical Physics Letters, 2002, 363, 523-528.	2.6	46
99	The effect of the symmetric and asymmetric stretching vibrations on the CH3D+O(3P)â†'CH3+OD reaction. Chemical Physics Letters, 2002, 363, 529-533.	2.6	22
100	Chemical Reactions. , 2002, , 1068-1080.		1
101	Time-Dependent Quantum Mechanical Calculations on the Formation of Molecular Hydrogen on a Graphite Surface via an Eleyâ^'Rideal Mechanismâ€. Journal of Physical Chemistry A, 2001, 105, 2173-2182.	2.5	84
102	Diffusion Monte Carlo simulations on uracilâ€"water using an anisotropic atomâ€"atom potential model. Faraday Discussions, 2001, 118, 95-108.	3.2	20
103	A Quantum Study on the Reaction between C(3P) and Acetyleneâ€. Journal of Physical Chemistry A, 2001, 105, 2694-2707.	2.5	36
104	Non-orthogonal basis sets for hyperspherical coordinate calculations on chemical reactions. Chemical Physics Letters, 2001, 346, 149-154.	2.6	2
105	Torsional diffusion Monte Carlo: A method for quantum simulations of proteins. Journal of Chemical Physics, 2001, 114, 9725-9732.	3.0	30
106	Improving reduced dimensionality quantum reaction dynamics with a generalized transition state. Application to CH4+O(3P). Journal of Chemical Physics, 2001, 115, 2188-2197.	3.0	34
107	Formation of molecular hydrogen on a graphite surface via an Eleyâ€"Rideal mechanism. Chemical Physics Letters, 2000, 319, 303-308.	2.6	97
108	Ab initio calculations on indoleâ€"water, 1-methylindoleâ€"water and indoleâ€"(water)2. Chemical Physics Letters, 2000, 331, 253-261.	2.6	40

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109	Perspective on "Quantum mechanical reactive scattering for three-dimensional atom plus diatom systems. II. Accurate cross sections for H + H 2 ". Theoretical Chemistry Accounts, 2000, 103, 326-327.	1.4	0
110	Mechanism of Photoinduced Changes in the Structure and Optical Properties of AmorphousAs2S3. Physical Review Letters, 2000, 85, 3305-3308.	7.8	40
111	Quaternion formulation of diffusion quantum Monte Carlo for the rotation of rigid molecules in clusters. Journal of Chemical Physics, 2000, 113, 5193.	3.0	26
112	A quantum model Hamiltonian to treat reactions of the type X+YCZ3â†'XY+CZ3: Application to O(3P)+CH4â†'OH+CH3. Journal of Chemical Physics, 2000, 112, 1859-1867.	3.0	112
113	Ab initio and diffusion Monte Carlo study of uracilâ€"water, thymineâ€"water, cytosineâ€"water, and cytosineâ€"(water)2. Physical Chemistry Chemical Physics, 2000, 2, 1281-1290.	2.8	88
114	Quantum scattering and quasi-classical trajectory calculations for the H2+OH â‡Œ H2O+H reaction on a new potential surface. Physical Chemistry Chemical Physics, 2000, 2, 693-700.	2.8	86
115	The effect of the symmetric and asymmetric stretching vibrations of CH4 on the O(3P) + CH4â†'OH + CH3 reaction. Physical Chemistry Chemical Physics, 2000, 2, 4105-4114.	2.8	35
116	H-Densities:â€‰ A New Concept for Hydrated Molecules. Accounts of Chemical Research, 2000, 33, 441-447.	15.6	55
117	Quantum Simulation of Phenolâ^'Water Clusters. Journal of Physical Chemistry A, 2000, 104, 5590-5599.	2.5	48
118	Simulation of Water Clusters with Rigid-Body Diffusion Monte Carlo. , 2000, , 187-199.		0
119	Perspective on â€œQuantum mechanical reactive scattering for three-dimensional atom plus diatom systems. II. Accurate cross sections for H + H2â€• , 2000, , 326-327.		0
120	A Quantum Model Hamiltonian to Study X + YCZ3 â†" XY + CZ3 Reactions. Lecture Notes in Quantum Chemistry II, 2000, , 286-290.	0.3	0
121	Quantum Dynamics of Gas-Phase S N 2 Reactions. Lecture Notes in Quantum Chemistry II, 2000, , 299-302.	0.3	0
122	A noninvasive rf probe for the study of ionization and dissociation processes in technological plasmas. Journal of Applied Physics, 1999, 86, 4100-4106.	2.5	6
123	Diffusion Monte Carlo simulations of the dipole-bound state of the water dimer anion. Journal of Chemical Physics, 1999, 111, 10559-10565.	3.0	23
124	Quantum mechanical study of the vibrational relaxation of O2+ colliding with Kr. Journal of Chemical Physics, 1999, 111, 1972-1978.	3.0	4
125	Isotopic branching in (He,â€ŠHD+) collisions: A time-dependent quantum mechanical study in three dimensions. Journal of Chemical Physics, 1999, 111, 10910-10918.	3.0	30
126	Diffusion Monte Carlo simulations of methanolâ€"water clusters. Chemical Physics Letters, 1999, 301, 275-280.	2.6	21

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127	CHEMICAL PHYSICS:Interfering with Water. Science, 1999, 285, 1218-1219.	12.6	2
128	Mode-selective decay dynamics of the ortho-H₂â€”OH complex: experiment and theory. Molecular Physics, 1999, 97, 151-158.	1.7	4
129	Quantum dynamics of the O(3P)+CH4â†'CH3+OH reaction. Physical Chemistry Chemical Physics, 1999, 1, 1173-1179.	2.8	66
130	Quantum scattering calculations on the SN2 reaction Clâ¯+CH3Brâ†'ClCH3+Brâ¯. Journal of Chemical Physics, 1999, 110, 9483-9491.	3.0	38
131	Quantum stereodynamics of four-atom reactions: theory and application to H2+OHâ†"H2O+H. Faraday Discussions, 1999, 113, 119-132.	3.2	15
132	Time-dependent wavepacket study of the vibrational predissociation of He2Br2. PhysChemComm, 1999, 2, 5.	0.8	1
133	Quantum-mechanical study of the resonances of the SN2 reaction Cl-+CH3Clâ†'ClCH3+Cl-. Physical Chemistry Chemical Physics, 1999, 1, 1197-1203.	2.8	35
134	Ab Initio Calculations on Uracilâ¯Water. Journal of Physical Chemistry A, 1999, 103, 1611-1618.	2.5	119
135	Time-dependent wavepacket calculations on polyatomic reactive scattering. Computer Physics Communications, 1998, 108, 191-199.	7.5	3
136	Speed improvement of diffusion quantum Monte Carlo calculations on weakly bound clusters. Chemical Physics Letters, 1998, 283, 269-276.	2.6	23
137	Time-resolved dissociation of the H2â€“OH entrance channel complex. Chemical Physics Letters, 1998, 294, 518-522.	2.6	8
138	New Potential Energy Function for Four-Atom Reactions. Application to OH + H2. Journal of Physical Chemistry A, 1998, 102, 9631-9637.	2.5	98
139	Quantum Theory of Chemical Reaction Dynamics. Science, 1998, 279, 1879-1882.	12.6	149
140	Reactive scattering of highly vibrationally excited oxygen molecules: Ozone formation?. Journal of Chemical Physics, 1998, 108, 3566-3573.	3.0	42
141	Quantum scattering on SN2 reactions: Influence of azimuthal rotations. Journal of Chemical Physics, 1998, 109, 8200-8217.	3.0	52
142	Using quantum rotational polarization moments to describe the stereodynamics of the H+D2(v=0,j=0)â†'HD(vâ€²,jâ€²)+D reaction. Journal of Chemical Physics, 1998, 108, 3142-3153.	3.0	94
143	Vibrational predissociation of D2HF and H2HF with a new potential energy surface. Molecular Physics, 1998, 93, 619-625.	1.7	11
144	Diffusion Monte Carlo studies of water clusters. Advances in Molecular Vibrations and Collision Dynamics, 1998, , 311-363.	0.8	7

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145	Quantum dynamics of the Walden inversion reaction Clâ¯'+CH3Clâ†'ClCH3+Clâ¯'. Journal of Chemical Physics, 1997, 106, 575-583.	3.0	92
146	Classical and approximate quantum investigations of vibrational energy transfer in S1 p-difluorobenzene. Journal of Chemical Physics, 1997, 106, 5439-5453.	3.0	7
147	The C6H6â€"(H2O)2 complex: Theoretical predictions of the structure, energetics, and tunneling dynamics. Journal of Chemical Physics, 1997, 106, 849-863.	3.0	31
148	Temperature dependence of the rate constant for the Clâ¯'+CH3Br reaction down to 23 K. Journal of Chemical Physics, 1997, 107, 1021-1024.	3.0	63
149	Quantum theory of four-atom reactions using arrangement channel hyperspherical coordinates: Formulation and application to OH+H2â†"H2O+H. Journal of Chemical Physics, 1997, 107, 8975-8984.	3.0	93
150	Quasiclassicaltrajectorystudyof thereactionH2+OHâ†'H2O+H: Comparison with quantum results. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 841-846.	1.7	9
151	Influence of surface defects on the adsorption of HCl on ice. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 2763-2767.	1.7	63
152	Calculation of the photodetachment spectrum for H3O-. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 747-753.	1.7	12
153	Quantum dynamical stereochemistry of atomâ€"diatom reactions. Journal of Chemical Physics, 1997, 106, 4509-4521.	3.0	105
154	Theoretical Study of the Cage Water Hexamer Structure. Journal of Physical Chemistry A, 1997, 101, 6813-6819.	2.5	62
155	The Water Dipole Moment in Water Clusters. Science, 1997, 275, 814-817.	12.6	635
156	Calculations of rate constants for reactions of first and second row cations. Theoretical Chemistry Accounts, 1997, 98, 33-41.	1.4	7
157	Subsurface effects in the dissociation of H2 on Pd(111). Chemical Physics Letters, 1997, 266, 437-442.	2.6	6
158	The vibrational predissociation of HeBr2: a wavepacket study. Chemical Physics Letters, 1997, 271, 171-177.	2.6	10
159	Calculation of the vibrational spectral density of NO2 via density correlation functions. Chemical Physics Letters, 1997, 273, 55-61.	2.6	13
160	Combiningabinitiocomputations, neural networks, and diffusion Monte Carlo: An efficient method to treat weakly bound molecules. Journal of Chemical Physics, 1996, 105, 7597-7604.	3.0	135
161	Molecules on Ice. Science, 1996, 271, 1509-1509.	12.6	39
162	Structure of Water Clusters. The Contribution of Many-Body Forces, Monomer Relaxation, and Vibrational Zero-Point Energy. The Journal of Physical Chemistry, 1996, 100, 18014-18022.	2.9	245

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163	Timeâ€dependent waveâ€packet studies on the sticking of HCl to an ice surface. Journal of Chemical Physics, 1996, 104, 5663-5673.	3.0	59
164	A method to calculate vibrational frequency shifts in heteroclusters: application to N2+â€“Hen. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 11-15.	1.7	9
165	The dynamics of the reaction OH + D2 â†' HOD + D: Crossed beam experiments and quantum mechanical scattering calculations on ab initio potential energy surfaces. Chemical Physics, 1996, 207, 389-409.	1.9	114
166	A quenching method in quantum-classical studies of dynamics with a bifurcating wavefunction. Chemical Physics Letters, 1996, 262, 284-291.	2.6	25
167	Diffusion Monte Carlo studies of isotope-substituted water trimers. Chemical Physics Letters, 1996, 263, 680-686.	2.6	28
168	Characterization of a cage form of the water hexamer. Nature, 1996, 381, 501-503.	27.8	624
169	H2dissociation on metal surfaces: Sixâ€dimensional approximate quantum calculations. Journal of Chemical Physics, 1996, 105, 5258-5264.	3.0	19
170	Tunneling dynamics in water tetramer and pentamer. Journal of Chemical Physics, 1996, 105, 6626-6633.	3.0	85
171	Fourâ€center reactions: A quantal model for H4. Journal of Chemical Physics, 1996, 104, 8413-8423.	3.0	30
172	Quantum simulation of the benzene-water complex. Molecular Physics, 1996, 88, 33-52.	1.7	62
173	Reactions of strongly polar ions with molecules. Chemical Physics Letters, 1995, 232, 267-272.	2.6	21
174	Quantum simulation of weakly bound complexes using direct ab initio energy points. Chemical Physics Letters, 1995, 237, 39-44.	2.6	16
175	Electronic spectra of the OH(A2Î£+)-H2 and OH(A2Î£+)-D2 complexes. Chemical Physics Letters, 1995, 244, 421-426.	2.6	12
176	Reduced-dimension quantum calculations for molecule-surface reactions. Chemical Physics Letters, 1995, 246, 399-404.	2.6	6
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