Stuart Althorpe

List of Publications by Year
in descending order

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55 papers	3,363 citations	126901 33 h-index	149686 56 g-index
56 all docs	56 docs citations	56 times ranked	1417 citing authors

#	Article	IF	Citations
1	QUANTUMSCATTERINGCALCULATIONS ONCHEMICALREACTIONS. Annual Review of Physical Chemistry, 2003, 54, 493-529.	10.8	371
2	Concerted hydrogen-bond breaking by quantum tunneling in the water hexamer prism. Science, 2016, 351, 1310-1313.	12.6	256
3	Ring-polymer molecular dynamics rate-theory in the deep-tunneling regime: Connection with semiclassical instanton theory. Journal of Chemical Physics, 2009, 131, 214106.	3.0	242
4	Observation and interpretation of a time-delayed mechanism in the hydrogen exchange reaction. Nature, 2002, 416, 67-70.	27.8	187
5	Quantum wavepacket method for state-to-state reactive cross sections. Journal of Chemical Physics, 2001, 114, 1601-1616.	3.0	152
6	Theoretical Study of Geometric Phase Effects in the Hydrogen-Exchange Reaction. Science, 2005, 309, 1227-1230.	12.6	141
7	Derivation of a true (t â†' 0+) quantum transition-state theory. I. Uniqueness and equivalence to ring-polymer molecular dynamics transition-state-theory. Journal of Chemical Physics, 2013, 138, 084108.	3.0	101
8	Ring-polymer instanton method for calculating tunneling splittings. Journal of Chemical Physics, 2011, 134, 054109.	3.0	98
9	On the equivalence of two commonly used forms of semiclassical instanton theory. Journal of Chemical Physics, 2011, 134, 114104.	3.0	93
10	Communication: Relation of centroid molecular dynamics and ring-polymer molecular dynamics to exact quantum dynamics. Journal of Chemical Physics, 2015, 142, 191101.	3.0	90
11	Boltzmann-conserving classical dynamics in quantum time-correlation functions: â€œMatsubara dynamicsâ€• Journal of Chemical Physics, 2015, 142, 134103.	3.0	89
12	Geometric phase effects in the H+H2 reaction: Quantum wave-packet calculations of integral and differential cross sections. Journal of Chemical Physics, 2005, 122, 204324.	3.0	86
13	General explanation of geometric phase effects in reactive systems: Unwinding the nuclear wave function using simple topology. Journal of Chemical Physics, 2006, 124, 084105.	3.0	85
14	Instanton calculations of tunneling splittings for water dimer and trimer. Journal of Chemical Physics, 2011, 135, 124109.	3.0	80
15	Calculation of the intermolecular bound states for water dimer. Journal of Chemical Physics, 1994, 101, 3603-3609.	3.0	77
16	Strong geometric-phase effects in the hydrogen-exchange reaction at high collision energies. Journal of Chemical Physics, 2008, 128, 124322.	3.0	74
17	Disagreement between theory and experiment in the simplest chemical reaction: Collision energy dependent rotational distributions for H+D2â†'HD(Î½â€²=3,jâ€²)+D. Journal of Chemical Physics, 2004, 120, 3244-3254.	3.0	62
18	Effect of the geometric phase on the dynamics of the hydrogen-exchange reaction. Journal of Chemical Physics, 2007, 126, 044317.	3.0	55

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19	Investigation of Terahertz Vibrationâ€“Rotation Tunneling Spectra for the Water Octamer. Journal of Physical Chemistry A, 2013, 117, 6960-6966.	2.5	52
20	Derivation of a true (t â†' 0+) quantum transition-state theory. II. Recovery of the exact quantum rate in the absence of recrossing. Journal of Chemical Physics, 2013, 139, 084115.	3.0	50
21	Time-dependent plane wave packet formulation of quantum scattering with application to H+D2â†'HD+D. Journal of Chemical Physics, 2002, 117, 4623-4627.	3.0	49
22	Quantum Tunneling Rates of Gas-Phase Reactions from On-the-Fly Instanton Calculations. Journal of Physical Chemistry Letters, 2016, 7, 4374-4379.	4.6	49
23	Effect of the geometric phase on nuclear dynamics at a conical intersection: Extension of a recent topological approach from one to two coupled surfaces. Journal of Chemical Physics, 2008, 129, 214117.	3.0	48
24	Non-equilibrium dynamics from RPMD and CMD. Journal of Chemical Physics, 2016, 145, 204118.	3.0	48
25	A new method for calculating the rovibrational states of polyatomics with application to water dimer. Journal of Chemical Physics, 1995, 102, 4390-4399.	3.0	41
26	On the role of the conical intersection in H+H2 reactive scattering. Chemical Physics Letters, 2003, 381, 743-750.	2.6	40
27	Shallow-tunnelling correction factor for use with Wignerâ€“Eyring transition-state theory. Physical Chemistry Chemical Physics, 2014, 16, 24292-24300.	2.8	38
28	Quantum Scattering with Energy-Filtered Plane Wave Packets:â€‰ Visualizing the F + HD â€œRidgeâ€• Mechanism. Journal of Physical Chemistry A, 2003, 107, 7152-7160.	2.5	36
29	Path-integral dynamics of water using curvilinear centroids. Journal of Chemical Physics, 2019, 151, .	3.0	36
30	Locating Instantons in Calculations of Tunneling Splittings: The Test Case of Malonaldehyde. Journal of Chemical Theory and Computation, 2016, 12, 787-803.	5.3	35
31	Collision energy dependence of the HD(Î½â€²=2) product rotational distribution of the H+D2 reaction in the range 1.30â€“1.89 eV. Journal of Chemical Physics, 2004, 120, 3255-3264.	3.0	34
32	Quantum tunneling splittings from path-integral molecular dynamics. Journal of Chemical Physics, 2016, 144, 114108.	3.0	34
33	Tunneling splittings from path-integral molecular dynamics using a Langevin thermostat. Journal of Chemical Physics, 2018, 148, 234102.	3.0	34
34	Which quantum statisticsâ€“classical dynamics method is best for water?. Faraday Discussions, 2019, 221, 350-366.	3.2	34
35	Tunneling Splittings in Water Clusters from Path Integral Molecular Dynamics. Journal of Physical Chemistry Letters, 2019, 10, 7300-7304.	4.6	32
36	Path-integral approximations to quantum dynamics. European Physical Journal B, 2021, 94, 1.	1.5	30

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37	On the uniqueness of t â†' 0+ quantum transition-state theory. Journal of Chemical Physics, 2013, 139, 084116.	3.0	27
38	Approximating Matsubara dynamics using the planetary model: Tests on liquid water and ice. Journal of Chemical Physics, 2018, 148, 102336.	3.0	27
39	Hunt for geometric phase effects in H + HD â†' HD(vâ€², jâ€²) + H. Journal of Chemical Physics, 2013, 139, 144316.	3.0	26
40	Strong geometric-phase effects in the hydrogen-exchange reaction at high collision energies: II. Quasiclassical trajectory analysis. Molecular Physics, 2010, 108, 969-980.	1.7	25
41	Rovibrational transitions of the methaneâ€“water dimer from intermolecular quantum dynamical computations. Physical Chemistry Chemical Physics, 2016, 18, 22816-22826.	2.8	24
42	Plane wave packet formulation of atom-plus-diatom quantum reactive scattering. Journal of Chemical Physics, 2004, 121, 1175-1186.	3.0	21
43	Differential Cross Sections for the H + D₂ â†' HD(vâ€² = 3, jâ€² = 4â€“10) + D Reaction above the Conical Intersection. Journal of Physical Chemistry A, 2015, 119, 12036-12042.	2.5	18
44	Calculating splittings between energy levels of different symmetry using path-integral methods. Journal of Chemical Physics, 2016, 144, 114109.	3.0	18
45	Mean-field Matsubara dynamics: Analysis of path-integral curvature effects in rovibrational spectra. Journal of Chemical Physics, 2018, 149, 014102.	3.0	18
46	Which Is Better at Predicting Quantum-Tunneling Rates: Quantum Transition-State Theory or Free-Energy Instanton Theory?. Journal of Physical Chemistry Letters, 2014, 5, 3976-3980.	4.6	16
47	On the â€œMatsubara heatingâ€•of overtone intensities and Fermi splittings. Journal of Chemical Physics, 2021, 155, 104107.	3.0	12
48	An alternative derivation of ring-polymer molecular dynamics transition-state theory. Journal of Chemical Physics, 2016, 144, 174107.	3.0	10
49	Path Integral Energy Landscapes for Water Clusters. Journal of Chemical Theory and Computation, 2019, 15, 33-42.	5.3	10
50	Influence of the Geometric Phase and Non-Adiabatic Couplings on the Dynamics of the H+H2 Molecular System. Springer Series in Chemical Physics, 2009, , 201-237.	0.2	10
51	Testing the quasicentroid molecular dynamics method on gas-phase ammonia. Journal of Chemical Physics, 2021, 155, 174120.	3.0	10
52	Simultaneous Measurement of Reactive and Inelastic Scattering: Differential Cross Section of the Hâ€¯+â€¯HDâ€¯â†'â€¯HD(vâ€²,â€¯jâ€²)â€¯+â€¯H Reaction. Zeitschrift Fur Physikalische Chemie, 2013, 227, .	2.8	8
53	Improved free-energy interpolation scheme for obtaining gas-phase reaction rates from ring-polymer molecular dynamics. Molecular Physics, 2012, 110, 875-883.	1.7	7
54	Setting the Trap for Reactive Resonances. Science, 2010, 327, 1460-1461.	12.6	6

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55	Symmetry Analysis of Geometric-Phase Effects in Quantum Dynamics. Advanced Series in Physical Chemistry, 2011, , 155-194.	1.5	1