Stuart Althorpe

List of Publications by Citations

56 papers	2,774 citations	29 h-index	52 g-index
56 ext. papers	3,107 ext. citations	6.3 avg, IF	5.62 L-index

#	Paper	IF	Citations
56	Quantum scattering calculations on chemical reactions. *Annual Review of Physical Chemistry*, **2003**, 54, 493-529	15.7	340
55	Ring-polymer molecular dynamics rate-theory in the deep-tunneling regime: Connection with semiclassical instanton theory. *Journal of Chemical Physics*, **2009**, 131, 214106	3.9	200
54	Concerted hydrogen-bond breaking by quantum tunneling in the water hexamer prism. *Science*, **2016**, 351, 1310-3	33.3	182
53	Observation and interpretation of a time-delayed mechanism in the hydrogen exchange reaction. *Nature*, **2002**, 416, 67-70	50.4	172
52	Quantum wavepacket method for state-to-state reactive cross sections. *Journal of Chemical Physics* , **2001**, 114, 1601-1616	3.9	140
51	Theoretical study of geometric phase effects in the hydrogen-exchange reaction. *Science*, **2005**, 309, 1227-30	33.3	124
50	Derivation of a true (t -> 0+) quantum transition-state theory. I. Uniqueness and equivalence to ring-polymer molecular dynamics transition-state-theory. *Journal of Chemical Physics*, **2013**, 138, 084108	3.9	88
49	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	3.9	79
48	Communication: Relation of centroid molecular dynamics and ring-polymer molecular dynamics to exact quantum dynamics. *Journal of Chemical Physics*, **2015**, 142, 191101	3.9	78
47	Ring-polymer instanton method for calculating tunneling splittings. *Journal of Chemical Physics*, **2011**, 134, 054109	3.9	76
46	Boltzmann-conserving classical dynamics in quantum time-correlation functions: "Matsubara dynamics". *Journal of Chemical Physics*, **2015**, 142, 134103	3.9	72
45	Calculation of the intermolecular bound states for water dimer. *Journal of Chemical Physics*, **1994**, 101, 3603-3609	3.9	72
44	On the equivalence of two commonly used forms of semiclassical instanton theory. *Journal of Chemical Physics*, **2011**, 134, 114104	3.9	71
43	Instanton calculations of tunneling splittings for water dimer and trimer. *Journal of Chemical Physics*, **2011**, 135, 124109	3.9	65
42	Disagreement between theory and experiment in the simplest chemical reaction: collision energy dependent rotational distributions for H + D2 --> HD(nu' = 3,j') + D. *Journal of Chemical Physics*, **2004**, 120, 3244-54	3.9	60
41	General explanation of geometric phase effects in reactive systems: Unwinding the nuclear wave function using simple topology. *Journal of Chemical Physics*, **2006**, 124, 084105	3.9	57
40	Strong geometric-phase effects in the hydrogen-exchange reaction at high collision energies. *Journal of Chemical Physics*, **2008**, 128, 124322	3.9	51

39	Time-dependent plane wave packet formulation of quantum scattering with application to H+D2->HD+D. *Journal of Chemical Physics*, **2002**, 117, 4623-4627	3.9	48
38	Investigation of terahertz vibration-rotation tunneling spectra for the water octamer. *Journal of Physical Chemistry A*, **2013**, 117, 6960-6	2.8	44
37	Derivation of a true (t -> 0+) quantum transition-state theory. II. Recovery of the exact quantum rate in the absence of recrossing. *Journal of Chemical Physics*, **2013**, 139, 084115	3.9	43
36	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	3.9	43
35	Quantum Tunneling Rates of Gas-Phase Reactions from On-the-Fly Instanton Calculations. *Journal of Physical Chemistry Letters*, **2016**, 7, 4374-4379	6.4	40
34	Non-equilibrium dynamics from RPMD and CMD. *Journal of Chemical Physics*, **2016**, 145, 204118	3.9	40
33	A new method for calculating the rovibrational states of polyatomics with application to water dimer. *Journal of Chemical Physics*, **1995**, 102, 4390-4399	3.9	37
32	On the role of the conical intersection in H+H2 reactive scattering. *Chemical Physics Letters*, **2003**, 381, 743-750	2.5	35
31	Collision energy dependence of the HD(nu' = 2) product rotational distribution of the H + D2 reaction in the range 1.30-1.89 eV. *Journal of Chemical Physics*, **2004**, 120, 3255-64	3.9	33
30	Quantum Scattering with Energy-Filtered Plane Wave Packets: Visualizing the F + HD Ridge Mechanism *Journal of Physical Chemistry A*, **2003**, 107, 7152-7160	2.8	33
29	Shallow-tunnelling correction factor for use with Wigner-Eyring transition-state theory. *Physical Chemistry Chemical Physics*, **2014**, 16, 24292-300	3.6	32
28	Effect of the geometric phase on the dynamics of the hydrogen-exchange reaction. *Journal of Chemical Physics*, **2007**, 126, 044317	3.9	31
27	Locating Instantons in Calculations of Tunneling Splittings: The Test Case of Malonaldehyde. *Journal of Chemical Theory and Computation*, **2016**, 12, 787-803	6.4	28
26	On the uniqueness of t -> 0+ quantum transition-state theory. *Journal of Chemical Physics*, **2013**, 139, 084116	3.9	26
25	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	24
24	Quantum tunneling splittings from path-integral molecular dynamics. *Journal of Chemical Physics*, **2016**, 144, 114108	3.9	24
23	Hunt for geometric phase effects in H + HD -> HD(v', j') + H. *Journal of Chemical Physics*, **2013**, 139, 144316	3.9	23
22	Which quantum statistics-classical dynamics method is best for water?. *Faraday Discussions*, **2019**, 221, 350-366	3.6	22

21	Approximating Matsubara dynamics using the planetary model: Tests on liquid water and ice. *Journal of Chemical Physics*, **2018**, 148, 102336	3.9	20
20	Rovibrational transitions of the methane-water dimer from intermolecular quantum dynamical computations. *Physical Chemistry Chemical Physics*, **2016**, 18, 22816-26	3.6	20
19	Path-integral dynamics of water using curvilinear centroids. *Journal of Chemical Physics*, **2019**, 151, 054109	3.9	20
18	Plane wave packet formulation of atom-plus-diatom quantum reactive scattering. *Journal of Chemical Physics*, **2004**, 121, 1175-86	3.9	20
17	Differential Cross Sections for the H + D2 -> HD(v' = 3, j' = 4-10) + D Reaction above the Conical Intersection. *Journal of Physical Chemistry A*, **2015**, 119, 12036-42	2.8	16
16	Tunneling splittings from path-integral molecular dynamics using a Langevin thermostat. *Journal of Chemical Physics*, **2018**, 148, 234102	3.9	16
15	Tunneling Splittings in Water Clusters from Path Integral Molecular Dynamics. *Journal of Physical Chemistry Letters*, **2019**, 10, 7300-7304	6.4	15
14	Which Is Better at Predicting Quantum-Tunneling Rates: Quantum Transition-State Theory or Free-Energy Instanton Theory?. *Journal of Physical Chemistry Letters*, **2014**, 5, 3976-80	6.4	15
13	Mean-field Matsubara dynamics: Analysis of path-integral curvature effects in rovibrational spectra. *Journal of Chemical Physics*, **2018**, 149, 014102	3.9	13
12	Calculating splittings between energy levels of different symmetry using path-integral methods. *Journal of Chemical Physics*, **2016**, 144, 114109	3.9	13
11	An alternative derivation of ring-polymer molecular dynamics transition-state theory. *Journal of Chemical Physics*, **2016**, 144, 174107	3.9	10
10	The Influence of the Geometric Phase on Reaction Dynamics. *Advances in Chemical Physics*, **2008**, 1-42		9
9	Path-integral approximations to quantum dynamics. *European Physical Journal B*, **2021**, 94, 1	1.2	9
8	Path Integral Energy Landscapes for Water Clusters. *Journal of Chemical Theory and Computation*, **2019**, 15, 33-42	6.4	9
7	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	0.3	8
6	Simultaneous Measurement of Reactive and Inelastic Scattering: Differential Cross Section of the H + HD -> HD(v?, j?) + H Reaction. *Zeitschrift Fur Physikalische Chemie*, **2013**, 227,	3.1	7
5	On the "Matsubara heating" of overtone intensities and Fermi splittings. *Journal of Chemical Physics*, **2021**, 155, 104107	3.9	7
4	Improved free-energy interpolation scheme for obtaining gas-phase reaction rates from ring-polymer molecular dynamics. *Molecular Physics*, **2012**, 110, 875-883	1.7	5

3	Chemistry. Setting the trap for reactive resonances. *Science*, **2010**, 327, 1460-1	33.3	4
2	Testing the quasicentroid molecular dynamics method on gas-phase ammonia. *Journal of Chemical Physics*, **2021**, 155, 174120	3.9	4
1	Symmetry Analysis of Geometric-Phase Effects in Quantum Dynamics. *Advanced Series in Physical Chemistry*, **2011**, 155-194		1