Jeremy O Richardson

List of Publications by Year
in descending order

60	2,616	172457	189892
papers	citations	29 h-index	50 g-index

62	62	62	1630
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Concerted hydrogen-bond breaking by quantum tunneling in the water hexamer prism. Science, 2016, 351, 1310-1313.	12.6	256
2	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
3	i-PI 2.0: A universal force engine for advanced molecular simulations. Computer Physics Communications, 2019, 236, 214-223.	7.5	220
4	Communication: Nonadiabatic ring-polymer molecular dynamics. Journal of Chemical Physics, 2013, 139, 031102.	3.0	115
5	Ring-polymer instanton method for calculating tunneling splittings. Journal of Chemical Physics, 2011, 134, 054109.	3.0	98
6	Nanometre-scale spectroscopic visualization of catalytic sites during a hydrogenation reaction on a Pd/Au bimetallic catalyst. Nature Catalysis, 2020, 3, 834-842.	34.4	84
7	Instanton calculations of tunneling splittings for water dimer and trimer. Journal of Chemical Physics, 2011, 135, 124109.	3.0	80
8	Derivation of instanton rate theory from first principles. Journal of Chemical Physics, 2016, 144, 114106.	3.0	76
9	Perspective: Ring-polymer instanton theory. Journal of Chemical Physics, 2018, 148, 200901.	3.0	73
10	Ring-polymer instanton theory. International Reviews in Physical Chemistry, 2018, 37, 171-216.	2.3	68
11	Elucidating the Nuclear Quantum Dynamics of Intramolecular Double Hydrogen Transfer in Porphycene. Journal of the American Chemical Society, 2019, 141, 2526-2534.	13.7	68
12	Stress Test for Quantum Dynamics Approximations: Deep Tunneling in the Muonium Exchange Reaction D + HMu â†' DMu + H. Journal of Physical Chemistry Letters, 2014, 5, 4219-4224.	4.6	64
13	Ion-mediated hydrogen-bond rearrangement through tunnelling in the iodideâ€"dihydrate complex. Nature Chemistry, 2019, 11, 367-374.	13.6	55
14	Generalized spin mapping for quantum-classical dynamics. Journal of Chemical Physics, 2020, 152, 084110.	3.0	53
15	Investigation of Terahertz Vibrationâ€"Rotation Tunneling Spectra for the Water Octamer. Journal of Physical Chemistry A, 2013, 117, 6960-6966.	2.5	52
16	Spin-mapping approach for nonadiabatic molecular dynamics. Journal of Chemical Physics, 2019, 151, 044119.	3.0	52
17	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
18	Full- and reduced-dimensionality instanton calculations of the tunnelling splitting in the formic acid dimer. Physical Chemistry Chemical Physics, 2017, 19, 966-970.	2.8	49

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19	Ab initio instanton rate theory made efficient using Gaussian process regression. Faraday Discussions, 2018, 212, 237-258.	3.2	48
20	Simultaneous Deep Tunneling and Classical Hopping for Hydrogen Diffusion on Metals. Physical Review Letters, 2017, 119, 126001.	7.8	46
21	On the identity of the identity operator in nonadiabatic linearized semiclassical dynamics. Journal of Chemical Physics, 2019, 150, 071101.	3.0	46
22	Benchmarking Quasiclassical Mapping Hamiltonian Methods for Simulating Electronically Nonadiabatic Molecular Dynamics. Journal of Chemical Theory and Computation, 2020, 16, 2883-2895.	5.3	44
23	Semiclassical Greenâ€™s functions and an instanton formulation of electron-transfer rates in the nonadiabatic limit. Journal of Chemical Physics, 2015, 143, 134115.	3.0	40
24	An analysis of nonadiabatic ring-polymer molecular dynamics and its application to vibronic spectra. Chemical Physics, 2017, 482, 124-134.	1.9	40
25	Ring-polymer instanton theory of electron transfer in the nonadiabatic limit. Journal of Chemical Physics, 2015, 143, 134116.	3.0	39
26	Origins of fast diffusion of water dimers on surfaces. Nature Communications, 2020, 11, 1689.	12.8	39
27	Kinetic isotope effects and how to describe them. Structural Dynamics, 2017, 4, 061501.	2.3	37
28	Microcanonical and thermal instanton rate theory for chemical reactions at all temperatures. Faraday Discussions, 2016, 195, 49-67.	3.2	36
29	Improved population operators for multi-state nonadiabatic dynamics with the mixed quantum-classical mapping approach. Faraday Discussions, 2019, 221, 150-167.	3.2	33
30	Molecular-Level Insights on Reactive Arrangement in On-Surface Photocatalytic Coupling Reactions Using Tip-Enhanced Raman Spectroscopy. Journal of the American Chemical Society, 2022, 144, 538-546.	13.7	29
31	Instanton formulation of Fermiâ€™s golden rule in the Marcus inverted regime. Journal of Chemical Physics, 2020, 152, 034106.	3.0	27
32	A partially linearized spin-mapping approach for nonadiabatic dynamics. I. Derivation of the theory. Journal of Chemical Physics, 2020, 153, 194109.	3.0	26
33	Non-oscillatory flux correlation functions for efficient nonadiabatic rate theory. Journal of Chemical Physics, 2014, 141, 074106.	3.0	25
34	Quantum tunnelling pathways of the water pentamer. Physical Chemistry Chemical Physics, 2020, 22, 1035-1044.	2.8	23
35	A partially linearized spin-mapping approach for nonadiabatic dynamics. II. Analysis and comparison with related approaches. Journal of Chemical Physics, 2020, 153, 194110.	3.0	20
36	Effects of tunnelling and asymmetry for system-bath models of electron transfer. Journal of Chemical Physics, 2018, 148, 102311.	3.0	19

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37	Semiclassical instanton formulation of Marcusâ€“Levichâ€“Jortner theory. Journal of Chemical Physics, 2020, 152, 244117.	3.0	17
38	Spin Crossover of Thiophosgene via Multidimensional Heavy-Atom Quantum Tunneling. Journal of the American Chemical Society, 2021, 143, 20952-20961.	13.7	17
39	Explaining the Efficiency of Photosynthesis: Quantum Uncertainty or Classical Vibrations?. Journal of Physical Chemistry Letters, 2022, 13, 3392-3399.	4.6	16
40	Non-adiabatic reactions: general discussion. Faraday Discussions, 2016, 195, 311-344.	3.2	15
41	Nonadiabatic quantum transition-state theory in the golden-rule limit. I. Theory and application to model systems. Journal of Chemical Physics, 2019, 150, 104107.	3.0	15
42	A partially linearized spin-mapping approach for simulating nonlinear optical spectra. Journal of Chemical Physics, 2022, 156, 024108.	3.0	15
43	Instanton theory of tunneling in molecules with asymmetric isotopic substitutions. Journal of Chemical Physics, 2020, 153, 094101.	3.0	14
44	Semiclassical analysis of the quantum instanton approximation. Journal of Chemical Physics, 2019, 151, 144111.	3.0	12
45	Instanton theory for Fermiâ€™s golden rule and beyond. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2022, 380, 20200378.	3.4	12
46	Instanton calculations of tunneling splittings in chiral molecules. Journal of Computational Chemistry, 2021, 42, 210-221.	3.3	11
47	Heavyâ€Atom Quantum Tunnelling in Spin Crossovers of Nitrenes**. Angewandte Chemie - International Edition, 2022, 61, .	13.8	11
48	Calculations of quantum tunnelling rates for muonium reactions with methane, ethane and propane. Physical Chemistry Chemical Physics, 2020, 22, 16843-16854.	2.8	10
49	Microcanonical Tunneling Rates from Density-of-States Instanton Theory. Journal of Chemical Theory and Computation, 2021, 17, 40-55.	5.3	10
50	Quantum Tunnelling Driven H₂ Formation on Graphene. Journal of Physical Chemistry Letters, 2022, 13, 3173-3181.	4.6	10
51	Nonadiabatic quantum transition-state theory in the golden-rule limit. II. Overcoming the pitfalls of the saddle-point and semiclassical approximations. Journal of Chemical Physics, 2019, 151, 214101.	3.0	9
52	Quantum Entanglement from Classical Trajectories. Physical Review Letters, 2021, 127, 250403.	7.8	9
53	Nonadiabatic instanton rate theory beyond the golden-rule limit. Journal of Chemical Physics, 2022, 156, 174115.	3.0	9
54	Divide-and-Conquer Method for Instanton Rate Theory. Journal of Chemical Theory and Computation, 2019, 15, 2816-2825.	5.3	7

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55	Revisiting nuclear tunnelling in the aqueous ferrousâ€“ferric electron transfer. Physical Chemistry Chemical Physics, 2020, 22, 10687-10698.	2.8	7
56	Quantum Dynamics in Water Clusters. , 2021, , 301-326.		6
57	Tunnelling assisted hydrogen elimination mechanisms of FeCl3/TEMPO. Chemical Communications, 2022, 58, 565-568.	4.1	5
58	Understanding Chemical Reactions beyond Transition-State Theory. Chimia, 2018, 72, 309.	0.6	3
59	Quantum dynamics of isolated molecules: general discussion. Faraday Discussions, 2018, 212, 281-306.	3.2	0
60	Heavyâ€Atom Quantum Tunnelling in Spin Crossovers of Nitrenes. Angewandte Chemie, 0, , .	2.0	0