Dimitri Antoniou

List of Publications by Year
in descending order

45	1,389	257450	330143
papers	citations	24 h-index	37 g-index

47	47	47	784
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Internal Enzyme Motions as a Source of Catalytic Activity:Â Rate-Promoting Vibrations and Hydrogen Tunneling. Journal of Physical Chemistry B, 2001, 105, 5553-5558.	2.6	138
2	Barrier passage and protein dynamics in enzymatically catalyzed reactions. FEBS Journal, 2002, 269, 3103-3112.	0.2	137
3	Computational and Theoretical Methods to Explore the Relation between Enzyme Dynamics and Catalysis. Chemical Reviews, 2006, 106, 3170-3187.	47.7	116
4	Promoting Vibrations in Human Purine Nucleoside Phosphorylase. A Molecular Dynamics and Hybrid Quantum Mechanical/Molecular Mechanical Study. Journal of the American Chemical Society, 2004, 126, 15720-15729.	13.7	85
5	Activated chemistry in the presence of a strongly symmetrically coupled vibration. Journal of Chemical Physics, 1998, 108, 3620-3625.	3.0	56
6	Protein Dynamics and Enzymatic Chemical Barrier Passage. Journal of Physical Chemistry B, 2011, 115, 15147-15158.	2.6	48
7	Barrier crossing in dihydrofolate reductase does not involve a rate-promoting vibration. Molecular Physics, 2012, 110, 531-536.	1.7	48
8	Mass Modulation of Protein Dynamics Associated with Barrier Crossing in Purine Nucleoside Phosphorylase. Journal of Physical Chemistry Letters, 2012, 3, 3538-3544.	4.6	47
9	Modulating Enzyme Catalysis through Mutations Designed to Alter Rapid Protein Dynamics. Journal of the American Chemical Society, 2016, 138, 3403-3409.	13.7	44
10	A molecular dynamics quantum Kramers study of proton transfer in solution. Journal of Chemical Physics, 1999, 110, 465-472.	3.0	43
11	Toward Identification of the Reaction Coordinate Directly from the Transition State Ensemble Using the Kernel PCA Method. Journal of Physical Chemistry B, 2011, 115, 2465-2469.	2.6	43
12	Quantum proton transfer with spatially dependent friction: Phenol-amine in methyl chloride. Journal of Chemical Physics, 1999, 110, 7359-7364.	3.0	42
13	The stochastic separatrix and the reaction coordinate for complex systems. Journal of Chemical Physics, 2009, 130, 151103.	3.0	40
14	Electric Fields and Fast Protein Dynamics in Enzymes. Journal of Physical Chemistry Letters, 2017, 8, 6165-6170.	4.6	40
15	Insight into Catalytically Relevant Correlated Motions in Human Purine Nucleoside Phosphorylaseâ€. Journal of Physical Chemistry A, 2006, 110, 463-472.	2.5	35
16	Hydride Transfer in DHFR by Transition Path Sampling, Kinetic Isotope Effects, and Heavy Enzyme Studies. Biochemistry, 2016, 55, 157-166.	2.5	35
17	Optimization of the Turnover in Artificial Enzymes via Directed Evolution Results in the Coupling of Protein Dynamics to Chemistry. Journal of the American Chemical Society, 2019, 141, 10431-10439.	13.7	33
18	Slow Conformational Motions That Favor Sub-picosecond Motions Important for Catalysis. Journal of Physical Chemistry B, 2010, 114, 15985-15990.	2.6	32

#	Article	IF	Citations
19	Nuclear-spin relaxation and spin-wave collective modes in a disordered two-dimensional electron gas. Physical Review B, 1991, 43, 11686-11693.	3.2	30
20	The Promoting Vibration in Human Heart Lactate Dehydrogenase Is a Preferred Vibrational Channel. Journal of Physical Chemistry B, 2011, 115, 15439-15444.	2.6	30
21	Proton transfer in benzoic acid crystals: Another look using quantum operator theory. Journal of Chemical Physics, 1998, 109, 2287-2293.	3.0	29
22	Transition path sampling study of classical rate-promoting vibrations. Journal of Chemical Physics, 2004, 121, 6442-6447.	3.0	28
23	Another Look at the Mechanisms of Hydride Transfer Enzymes with Quantum and Classical Transition Path Sampling. Journal of Physical Chemistry Letters, 2015, 6, 1177-1181.	4.6	26
24	Catalytic-site design for inverse heavy-enzyme isotope effects in human purine nucleoside phosphorylase. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 6456-6461.	7.1	24
25	Inverse enzyme isotope effects in human purine nucleoside phosphorylase with heavy asparagine labels. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E6209-E6216.	7.1	18
26	Nonadiabatic effects in a method that combines classical and quantum mechanics. Journal of Chemical Physics, 1996, 104, 3526-3530.	3.0	15
27	Nonequilibrium Solvation and the Quantum Kramers Problem:Â Proton Transfer in Aqueous Glycineâ€. Journal of Physical Chemistry A, 2001, 105, 2563-2567.	2.5	15
28	Magnetoplasmons and cyclotron resonance in disordered two-dimensional electronic systems. Physical Review B, 1992, 46, 15225-15232.	3.2	11
29	Incorporating Fast Protein Dynamics into Enzyme Design: A Proposed Mutant Aromatic Amine Dehydrogenase. Journal of Physical Chemistry B, 2017, 121, 7290-7298.	2.6	11
30	Approximate inclusion of quantum effects in transition path sampling. Journal of Chemical Physics, 2009, 131, 224111.	3.0	10
31	Enzyme Homologues Have Distinct Reaction Paths through Their Transition States. Journal of Physical Chemistry B, 2015, 119, 3662-3668.	2.6	10
32	Vibrational energy transfer in linear hydrocarbon chains: New quantum results. Journal of Chemical Physics, 1995, 103, 7277-7286.	3.0	9
33	Collective oscillations in a disordered two-dimensional electron gas at strong magnetic fields. Physical Review B, 1990, 41, 5440-5443.	3.2	8
34	Phase Space Bottlenecks in Enzymatic Reactions. Journal of Physical Chemistry B, 2016, 120, 433-439.	2.6	8
35	Inverse heavy enzyme isotope effects in methylthioadenosine nucleosidases. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	8
36	Temperature dependent spectral densities and quantum activated rate theory. Journal of Chemical Physics, 1998, 109, 5487-5492.	3.0	6

#	Article	IF	Citations
37	Effect of enzyme dynamics on catalytic activity. Advances in Physical Organic Chemistry, 2006, 41, 315-362.	0.5	6
38	New mixed quantumâ^•semiclassical propagation method. Journal of Chemical Physics, 2007, 126, 184107.	3.0	6
39	Role of Protein Motions in Catalysis by Formate Dehydrogenase. Journal of Physical Chemistry B, 2020, 124, 9483-9489.	2.6	6
40	Reply to â€œComment on 'Toward Identification of the Reaction Coordinate Directly from the Transition State Ensemble Using the Kernel PCA Method'â€• Journal of Physical Chemistry B, 2011, 115, 12674-12675.	2.6	5
41	Langevin equation in momentum space. Journal of Chemical Physics, 2003, 119, 11329-11334.	3.0	3
42	Harmonic collective modes in atomic liquids. Journal of Chemical Physics, 2001, 115, 4670-4675.	3.0	2
43	Linking Protein Dynamics to Enzyme Catalysis. , 2020, , 578-588.		2
44	Low-Frequency Collective Motions in Proteins. Journal of Theoretical and Computational Chemistry, 2003, 02, 163-169.	1.8	1
45	Method for Identifying Common Features in Reactive Trajectories of a Transition Path Sampling Ensemble. Journal of Chemical Theory and Computation, 2022, 18, 3997-4004.	5.3	0