Julian Echave

List of Publications by Year
in descending order

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67	3,046	186265	175258
papers	citations	28 h-index	52 g-index

74	74	74	2400
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Potential optimized discrete variable representation. Chemical Physics Letters, 1992, 190, 225-230.	2.6	567
2	Causes of evolutionary rate variation among protein sites. Nature Reviews Genetics, 2016, 17, 109-121.	16.3	247
3	The interface of protein structure, protein biophysics, and molecular evolution. Protein Science, 2012, 21, 769-785.	7.6	188
4	Gamma carbonic anhydrases in plant mitochondria. Plant Molecular Biology, 2004, 55, 193-207.	3.9	124
5	Measuring and comparing structural fluctuation patterns in large protein datasets. Bioinformatics, 2012, 28, 2431-2440.	4.1	111
6	Biophysical Models of Protein Evolution: Understanding the Patterns of Evolutionary Sequence Divergence. Annual Review of Biophysics, 2017, 46, 85-103.	10.0	103
7	Quantum theory of planar fourâ€atom reactions. Journal of Chemical Physics, 1994, 100, 402-422.	3.0	99
8	Functional Sites Induce Long-Range Evolutionary Constraints in Enzymes. PLoS Biology, 2016, 14, e1002452.	5.6	94
9	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
10	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
11	Evolutionary conservation of protein vibrational dynamics. Gene, 2008, 422, 7-13.	2.2	85
12	Evolutionary Conservation of Protein Backbone Flexibility. Journal of Molecular Evolution, 2006, 63, 448-457.	1.8	83
13	Delay Model of the Circadian Pacemaker. Journal of Theoretical Biology, 2000, 204, 565-573.	1.7	71
14	Site-Specific Structural Constraints on Protein Sequence Evolutionary Divergence: Local Packing Density versus Solvent Exposure. Molecular Biology and Evolution, 2014, 31, 135-139.	8.9	70
15	A mechanistic stress model of protein evolution accounts for site-specific evolutionary rates and their relationship with packing density and flexibility. BMC Evolutionary Biology, 2014, 14, 78.	3.2	68
16	Gamma carbonic anhydrase like complex interact with plant mitochondrial complex I. Plant Molecular Biology, 2004, 56, 947-957.	3.9	66
17	Exploring the Common Dynamics of Homologous Proteins. Application to the Globin Family. Biophysical Journal, 2005, 89, 3-13.	0.5	66
18	Relationship between protein thermodynamic constraints and variation of evolutionary rates among sites. Physical Biology, 2015, 12, 025002.	1.8	49

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19	A perturbative view of protein structural variation. Proteins: Structure, Function and Bioinformatics, 2010, 78, 173-180.	2.6	47
20	Local Packing Density Is the Main Structural Determinant of the Rate of Protein Sequence Evolution at Site Level. BioMed Research International, 2014, 2014, 1-10.	1.9	46
21	Evolutionary divergence of protein structure: The linearly forced elastic network model. Chemical Physics Letters, 2008, 457, 413-416.	2.6	45
22	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
23	Too packed to change: side-chain packing and site-specific substitution rates in protein evolution. PeerJ, 2015, 3, e911.	2.0	44
24	Site-Specific Amino Acid Replacement Matrices from Structurally Constrained Protein Evolution Simulations. Molecular Biology and Evolution, 2002, 19, 352-356.	8.9	41
25	What evolution tells us about protein physics, and protein physics tells us about evolution. Current Opinion in Structural Biology, 2017, 42, 59-66.	5.7	40
26	Relaxation Dynamics of Tryptophan in Water: A UV Fluorescence Up-Conversion and Molecular Dynamics Study. Journal of Physical Chemistry A, 2010, 114, 9034-9042.	2.5	31
27	A theoretical study of photofragmentation and geminate recombination of ICN in solid Ar. Journal of Chemical Physics, 1998, 109, 2844-2850.	3.0	30
28	Beyond Stability Constraints: A Biophysical Model of Enzyme Evolution with Selection on Stability and Activity. Molecular Biology and Evolution, 2019, 36, 613-620.	8.9	30
29	Sequence Determinants of Quaternary Structure in Lumazine Synthase. Molecular Biology and Evolution, 2004, 21, 97-107.	8.9	28
30	Why are the low-energy protein normal modes evolutionarily conserved?. Pure and Applied Chemistry, 2012, 84, 1931-1937.	1.9	26
31	Generality of the Structurally Constrained Protein Evolution model: assessment on representatives of the four main fold classes. Gene, 2005, 345, 45-53.	2.2	24
32	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
33	Sulfide-Binding Hemoglobins: Effects of Mutations on Active-Site Flexibility. Biophysical Journal, 2006, 91, 1698-1709.	0.5	21
34	Hybrid quantum/classical study of ICN in an Ar matrix: Photofragmentation and cage exit. Journal of Chemical Physics, 2000, 113, 1027-1034.	3.0	19
35	Evolutionary Analysis of Î³-Carbonic Anhydrase and Structurally Related Proteins. Molecular Phylogenetics and Evolution, 2000, 14, 323-334.	2.7	17
36	The structurally constrained protein evolution model accounts for sequence patterns of the LbetaH superfamily. BMC Evolutionary Biology, 2004, 4, 41.	3.2	17

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37	Dynactins p25 and p27 are predicted to adopt the LÎ²H fold. FEBS Letters, 2004, 562, 1-4.	2.8	15
38	Calculation of vibrational transition probabilities in molecular collisions: A recursive algebraic procedure. Journal of Chemical Physics, 1989, 91, 924-928.	3.0	14
39	Theoretical study of the solvatochromism of a merocyanine dye. Chemical Physics, 1997, 223, 183-194.	1.9	13
40	Caging and excited state emission of ICN trapped in cryogenic matrices: experiment and theory. Physical Chemistry Chemical Physics, 2000, 2, 4131-4138.	2.8	13
41	Quaternary Structure Constraints on Evolutionary Sequence Divergence. Molecular Biology and Evolution, 2006, 24, 349-351.	8.9	12
42	Computational characterisation of potential RNA-binding sites in arenavirus nucleocapsid proteins. Virus Genes, 1996, 13, 247-254.	1.6	11
43	Vibrational coherence and nonadiabatic dynamics in the condensed phase. Journal of Chemical Physics, 2002, 116, 3343-3352.	3.0	11
44	Molecular transition probabilities for time-dependent, bilinear Hamiltonians in many dimensions: A recursive procedure. Physical Review A, 1989, 40, 74-79.	2.5	9
45	A generalized intermediate picture of quantal time evolution using operator algebraic methods. Application to translationalâ€“vibrational energy transfer in molecular collisions. Journal of Chemical Physics, 1991, 94, 3537-3541.	3.0	9
46	Quasiclassicaltrajectorystudyof thereactionH2+OHâ†'H2O+H: Comparison with quantum results. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 841-846.	1.7	9
47	Molecular Dynamics Study of the Active Site of Methylamine Dehydrogenase. Journal of Physical Chemistry B, 2006, 110, 11592-11599.	2.6	9
48	The variation among sites of protein structure divergence is shaped by mutation and scaled by selection. Current Research in Structural Biology, 2020, 2, 156-163.	2.2	9
49	Quantum study of the structure of the active site of methylamine dehydrogenase. International Journal of Quantum Chemistry, 2005, 105, 937-945.	2.0	8
50	The magnus expansion for the damped harmonic oscillator. Chemical Physics, 1987, 117, 101-104.	1.9	6
51	Timeâ€dependent reactive scattering in hyperspherical coordinates: A close coupled wave packet approach. Journal of Chemical Physics, 1996, 104, 1380-1386.	3.0	6
52	(Too Many) Mathematical Models of Circadian Clocks (?). Biological Rhythm Research, 2001, 32, 285-298.	0.9	6
53	Simulations of the absorption band of the D-state of Hg2 in rare gas matrices. Chemical Physics Letters, 2003, 367, 651-656.	2.6	6
54	Evolutionary coupling range varies widely among enzymes depending on selection pressure. Biophysical Journal, 2021, 120, 4320-4324.	0.5	5

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55	On the convergence of the Magnus expansion in the SchrÃ¶dinger representation. Journal of Mathematical Physics, 1990, 31, 338-341.	1.1	4
56	On the bilinear approximation for timeâ€dependent Hamiltonians. Journal of Chemical Physics, 1990, 92, 1188-1193.	3.0	4
57	The planar reaction OH+H2â†'H2O+H: A quasiclassical trajectory study. Journal of Chemical Physics, 1996, 104, 2841-2846.	3.0	4
58	Quasi-classical rate constants for the inelastic process O 2 (Ï... i much greater than 1) + O 2 â†' O 2 (Ï... f) + O 2. Molecular Physics, 2000, 98, 1729-1735.	1.7	4
59	On the evolutionary conservation of protein dynamics. Physics of Life Reviews, 2013, 10, 31-32.	2.8	3
60	Construction of effective Hamiltonians for timeâ€dependent phenomena from variational principles. Journal of Chemical Physics, 1991, 95, 3607-3613.	3.0	2
61	Baker-Campbell-Hausdorff relations for finite-dimensional lie algebras. Journal of Mathematical Chemistry, 1992, 9, 87-94.	1.5	2
62	Assessing local structural perturbations in proteins. BMC Bioinformatics, 2005, 6, 226.	2.6	2
63	Teaching noncovalent interactions using protein molecular evolution. Biochemistry and Molecular Biology Education, 2008, 36, 284-286.	1.2	1
64	Fast computational mutation-response scanning of proteins. PeerJ, 2021, 9, e11330.	2.0	1
65	Rotationally and vibrationally inelastic scattering of 41 D2CO. Chemical Physics, 1992, 163, 339-349.	1.9	0
66	An analytical Fourier transform method for semiclassical quantization. Chemical Physics Letters, 1997, 270, 206-210.	2.6	0
67	The Quitel-2002. Theoretical Chemistry Accounts, 2003, 110, 359-359.	1.4	0