Ravindra Venkatramani

List of Publications by Year
in descending order

43	1,256	471509 17	361022 35
papers	citations	h-index	g-index

49	49	49	1630
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Role of Ligand Binding Site in Modulating the Mechanical Stability of Proteins with Î²-Grasp Fold. Journal of Physical Chemistry B, 2021, 125, 1009-1019.	2.6	3
2	Estimating the Directional Flexibility of Proteins from Equilibrium Thermal Fluctuations. Journal of Chemical Theory and Computation, 2021, 17, 3103-3118.	5.3	4
3	Identification of a copper ion recognition peptide sequence in the subunit II of cytochrome c oxidase: a combined theoretical and experimental study. Journal of Biological Inorganic Chemistry, 2021, 26, 411-425.	2.6	4
4	Multiscale modelling reveals higher charge transport efficiencies of DNA relative to RNA independent of mechanism. Nanoscale, 2020, 12, 18750-18760.	5.6	10
5	Transient Raman Snapshots of the Twisted Intramolecular Charge Transfer State in a Stilbazolium Dye. Journal of Physical Chemistry Letters, 2020, 11, 4842-4848.	4.6	17
6	Variance of Atomic Coordinates as a Dynamical Metric to Distinguish Proteins and Proteinâ€“Protein Interactions in Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2020, 124, 4247-4262.	2.6	4
7	Allosteric Regulation of Cyclin-B Binding by the Charge State of Catalytic Lysine in CDK1 Is Essential for Cell-Cycle Progression. Journal of Molecular Biology, 2019, 431, 2127-2142.	4.2	24
8	Ultrafast photoactivation of Câ”€H bonds inside water-soluble nanocages. Science Advances, 2019, 5, eaav4806.	10.3	41
9	UVâ€“Visible Lysineâ€“Glutamate Dimer Excitations in Protein Charge Transfer Spectra: TDDFT Descriptions Using an Optimally Tuned CAM-B3LYP Functional. Journal of Physical Chemistry B, 2019, 123, 10967-10979.	2.6	14
10	Differences in the mechanical unfolding pathways of apo- and copper-bound azurins. Scientific Reports, 2018, 8, 1989.	3.3	21
11	Optically sensing phospholipid induced coilâ€“helix transitions in the phosphoinositide-binding motif of gelsolin. Faraday Discussions, 2018, 207, 437-458.	3.2	5
12	Optical backbone-sidechain charge transfer transitions in proteins sensitive to secondary structure and modifications. Faraday Discussions, 2018, 207, 115-135.	3.2	17
13	Near UV-Visible electronic absorption originating from charged amino acids in a monomeric protein. Chemical Science, 2017, 8, 5416-5433.	7.4	136
14	Major Reaction Coordinates Linking Transient Amyloid-Î² Oligomers to Fibrils Measured at Atomic Level. Biophysical Journal, 2017, 113, 805-816.	0.5	32
15	Highlights from Kaleidoscope: A Discussion Meeting in Chemistry, Goa, India, July 2016. Chemical Communications, 2017, 53, 8926-8930.	4.1	0
16	Conductance in a bis-terpyridine based single molecular breadboard circuit. Chemical Science, 2017, 8, 1576-1591.	7.4	25
17	3.13 Computational Methods Related to Molecular Structure and Reaction Chemistry of Biomaterials â˜†. , 2017, , 245-267.		5
18	Organic photovoltaics and energy: general discussion. Faraday Discussions, 2014, 174, 341-355.	3.2	2

#	Article	IF	Citations
19	Breaking the simple proportionality between molecular conductances and charge transfer rates. Faraday Discussions, 2014, 174, 57-78.	3.2	44
20	The Single-Molecule Conductance and Electrochemical Electron-Transfer Rate Are Related by a Power Law. ACS Nano, 2013, 7, 5391-5401.	14.6	65
21	Protein structure quality assessment based on the distance profiles of consecutive backbone CÎ± atoms. F1000Research, 2013, 2, 211.	1.6	12
22	The electrostatic profile of consecutive CÎ² atoms applied to protein structure quality assessment. F1000Research, 2013, 2, 243.	1.6	5
23	The electrostatic profile of consecutive CÎ² atoms applied to protein structure quality assessment. F1000Research, 2013, 2, 243.	1.6	4
24	Effect of Backbone Flexibility on Charge Transfer Rates in Peptide Nucleic Acid Duplexes. Journal of the American Chemical Society, 2012, 134, 9335-9342.	13.7	38
25	Evidence for a Near-Resonant Charge Transfer Mechanism for Double-Stranded Peptide Nucleic Acid. Journal of the American Chemical Society, 2011, 133, 62-72.	13.7	45
26	Computational Methods Related to Reaction Chemistry. , 2011, , 155-169.		0
27	Nucleic acid charge transfer: Black, white and gray. Coordination Chemistry Reviews, 2011, 255, 635-648.	18.8	109
28	Computational delineation of the catalytic step of a highâ€fidelity DNA polymerase. Protein Science, 2010, 19, 815-825.	7.6	10
29	Optimizing Single-Molecule Conductivity of Conjugated Organic Oligomers with Carbodithioate Linkers. Journal of the American Chemical Society, 2010, 132, 7946-7956.	13.7	102
30	Is MD Geometry Sampling Sufficient for Nucleobase Electronic Structure Analysis of ET Reactions? Comparing Classical MD and QM/MM Methods. Journal of Physical Chemistry C, 2010, 114, 20496-20502.	3.1	13
31	Role of Nucleobase Energetics and Nucleobase Interactions in Single-Stranded Peptide Nucleic Acid Charge Transfer. Journal of the American Chemical Society, 2009, 131, 6498-6507.	13.7	55
32	Steering Electrons on Moving Pathways. Accounts of Chemical Research, 2009, 42, 1669-1678.	15.6	168
33	Photoconductivity and current-voltage characteristics of thin DNA films: experiments and modeling. , 2009, , .		1
34	Effect of oxidatively damaged DNA on the active site preorganization during nucleotide incorporation in a high fidelity polymerase from Bacillus stearothermophilus. Proteins: Structure, Function and Bioinformatics, 2008, 71, 1360-1372.	2.6	8
35	PNA versus DNA: Effects of Structural Fluctuations on Electronic Structure and Hole-Transport Mechanisms. Journal of the American Chemical Society, 2008, 130, 11752-11761.	13.7	112
36	Computational Study of the Force Dependence of Phosphoryl Transfer during DNA Synthesis by a High Fidelity Polymerase. Physical Review Letters, 2008, 100, 088102.	7.8	11

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37	Dephasing-Induced Vibronic Resonances in Difference Frequency Generation Spectroscopy. Journal of Physical Chemistry B, 2005, 109, 8132-8143.	2.6	17
38	Multidimensional Nonlinear Spectroscopy of Conformational Relaxation in Azobenzene Peptide. Springer Series in Chemical Physics, 2003, , 619-621.	0.2	0
39	Correlated line broadening in multidimensional vibrational spectroscopy. Journal of Chemical Physics, 2002, 117, 11089-11101.	3.0	60
40	Dipeptidyl peptidase-IV inhibitors used in type-2 diabetes inhibit a phospholipase C: a case of promiscuous scaffolds in proteins. F1000Research, 0, 2, 286.	1.6	8
41	The electrostatic profile of consecutive Cî² atoms applied to protein structure quality assessment. F1000Research, 0, 2, 243.	1.6	1
42	Promiscuous scaffolds in proteins - non-native, non-additive and non-trivial. F1000Research, 0, 2, 260.	1.6	0
43	PREMONITION - Preprocessing motifs in protein structures for search acceleration. F1000Research, 0, 3, 217.	1.6	3