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	Steering Electrons on Moving Pathways. Accounts of Chemical Research, 2009, 42, 1669-1678.	15.6	168
2	Near UV-Visible electronic absorption originating from charged amino acids in a monomeric protein. Chemical Science, 2017, 8, 5416-5433.	7.4	136
3	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
4	Nucleic acid charge transfer: Black, white and gray. Coordination Chemistry Reviews, 2011, 255, 635-648.	18.8	109
5	Optimizing Single-Molecule Conductivity of Conjugated Organic Oligomers with Carbodithioate Linkers. Journal of the American Chemical Society, 2010, 132, 7946-7956.	13.7	102
6	The Single-Molecule Conductance and Electrochemical Electron-Transfer Rate Are Related by a Power Law. ACS Nano, 2013, 7, 5391-5401.	14.6	65
7	Correlated line broadening in multidimensional vibrational spectroscopy. Journal of Chemical Physics, 2002, 117, 11089-11101.	3.0	60
8	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
9	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
10	Breaking the simple proportionality between molecular conductances and charge transfer rates. Faraday Discussions, 2014, 174, 57-78.	3.2	44
11	Ultrafast photoactivation of Câ”€H bonds inside water-soluble nanocages. Science Advances, 2019, 5, eaav4806.	10.3	41
12	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
13	Major Reaction Coordinates Linking Transient Amyloid-Î² Oligomers to Fibrils Measured at Atomic Level. Biophysical Journal, 2017, 113, 805-816.	0.5	32
14	Conductance in a bis-terpyridine based single molecular breadboard circuit. Chemical Science, 2017, 8, 1576-1591.	7.4	25
15	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
16	Differences in the mechanical unfolding pathways of apo- and copper-bound azurins. Scientific Reports, 2018, 8, 1989.	3.3	21
17	Dephasing-Induced Vibronic Resonances in Difference Frequency Generation Spectroscopy. Journal of Physical Chemistry B, 2005, 109, 8132-8143.	2.6	17
18	Optical backbone-sidechain charge transfer transitions in proteins sensitive to secondary structure and modifications. Faraday Discussions, 2018, 207, 115-135.	3.2	17

#	Article	IF	Citations
19	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
20	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
21	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
22	Protein structure quality assessment based on the distance profiles of consecutive backbone CÎ± atoms. F1000Research, 2013, 2, 211.	1.6	12
23	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
24	Computational delineation of the catalytic step of a highâ€fidelity DNA polymerase. Protein Science, 2010, 19, 815-825.	7.6	10
25	Multiscale modelling reveals higher charge transport efficiencies of DNA relative to RNA independent of mechanism. Nanoscale, 2020, 12, 18750-18760.	5.6	10
26	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
27	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
28	3.13 Computational Methods Related to Molecular Structure and Reaction Chemistry of Biomaterials â˜†. , 2017, , 245-267.		5
29	Optically sensing phospholipid induced coilâ€“helix transitions in the phosphoinositide-binding motif of gelsolin. Faraday Discussions, 2018, 207, 437-458.	3.2	5
30	The electrostatic profile of consecutive CÎ² atoms applied to protein structure quality assessment. F1000Research, 2013, 2, 243.	1.6	5
31	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
32	Estimating the Directional Flexibility of Proteins from Equilibrium Thermal Fluctuations. Journal of Chemical Theory and Computation, 2021, 17, 3103-3118.	5.3	4
33	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
34	The electrostatic profile of consecutive CÎ² atoms applied to protein structure quality assessment. F1000Research, 2013, 2, 243.	1.6	4
35	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
36	PREMONITION - Preprocessing motifs in protein structures for search acceleration. F1000Research, 0, 3, 217.	1.6	3

#	Article	IF	Citations
37	Organic photovoltaics and energy: general discussion. Faraday Discussions, 2014, 174, 341-355.	3.2	2
38	Photoconductivity and current-voltage characteristics of thin DNA films: experiments and modeling. , 2009, , .		1
39	The electrostatic profile of consecutive Cα² atoms applied to protein structure quality assessment. F1000Research, 0, 2, 243.	1.6	1
40	Computational Methods Related to Reaction Chemistry. , 2011, , 155-169.		0
41	Highlights from Kaleidoscope: A Discussion Meeting in Chemistry, Goa, India, July 2016. Chemical Communications, 2017, 53, 8926-8930.	4.1	0
42	Multidimensional Nonlinear Spectroscopy of Conformational Relaxation in Azobenzene Peptide. Springer Series in Chemical Physics, 2003, , 619-621.	0.2	0
43	Promiscuous scaffolds in proteins - non-native, non-additive and non-trivial. F1000Research, 0, 2, 260.	1.6	0