

Vijay S Pande

List of Publications by Year in descending order

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106
papers

17,923
citations

57758

44
h-index

32842

100
g-index

110
all docs

110
docs citations

110
times ranked

17409
citing authors

#	ARTICLE	IF	CITATIONS
1	Computational IR Spectroscopy of Insulin Dimer Structure and Conformational Heterogeneity. <i>Journal of Physical Chemistry B</i> , 2021, 125, 4620-4633.	2.6	14
2	A Targeted Computational Screen of the SWEETLEAD Database Reveals FDA-Approved Compounds with Anti-Dengue Viral Activity. <i>MBio</i> , 2020, 11, .	4.1	6
3	Dynamical model of the CLC-2 ion channel reveals conformational changes associated with selectivity-filter gating. <i>PLoS Computational Biology</i> , 2020, 16, e1007530.	3.2	9
4	Improvement in ADMET Prediction with Multitask Deep Featurization. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 8835-8848.	6.4	110
5	A modular DNA scaffold to study protein-protein interactions at single-molecule resolution. <i>Nature Nanotechnology</i> , 2019, 14, 988-993.	31.5	41
6	Synthesis of spiro-2,6-dioxopiperazine and spiro-2,6-dioxopyrazine scaffolds using amino acids in a three-component reaction to generate potential Sigma-1 (σ_1) receptor selective ligands. <i>European Journal of Medicinal Chemistry</i> , 2019, 164, 241-251.	5.5	5
7	Intradomain Interactions in an NMDA Receptor Fragment Mediate N-Glycan Processing and Conformational Sampling. <i>Structure</i> , 2019, 27, 55-65.e3.	3.3	9
8	Theoretical restrictions on longest implicit time scales in Markov state models of biomolecular dynamics. <i>Journal of Chemical Physics</i> , 2018, 148, 044111.	3.0	4
9	A Minimum Variance Clustering Approach Produces Robust and Interpretable Coarse-Grained Models. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1071-1082.	5.3	16
10	Markov State Models: From an Art to a Science. <i>Journal of the American Chemical Society</i> , 2018, 140, 2386-2396.	13.7	573
11	REDOR NMR Reveals Multiple Conformers for a Protein Kinase C Ligand in a Membrane Environment. <i>ACS Central Science</i> , 2018, 4, 89-96.	11.3	28
12	MoleculeNet: a benchmark for molecular machine learning. <i>Chemical Science</i> , 2018, 9, 513-530.	7.4	1,261
13	Transfer Learning from Markov Models Leads to Efficient Sampling of Related Systems. <i>Journal of Physical Chemistry B</i> , 2018, 122, 5291-5299.	2.6	14
14	Perspective: Computational chemistry software and its advancement as illustrated through three grand challenge cases for molecular science. <i>Journal of Chemical Physics</i> , 2018, 149, 180901.	3.0	72
15	Note: Variational encoding of protein dynamics benefits from maximizing latent autocorrelation. <i>Journal of Chemical Physics</i> , 2018, 149, 216101.	3.0	7
16	Bayesian analysis of isothermal titration calorimetry for binding thermodynamics. <i>PLoS ONE</i> , 2018, 13, e0203224.	2.5	24
17	PotentialNet for Molecular Property Prediction. <i>ACS Central Science</i> , 2018, 4, 1520-1530.	11.3	278
18	Automated design of collective variables using supervised machine learning. <i>Journal of Chemical Physics</i> , 2018, 149, 094106.	3.0	98

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19	Solving the RNA design problem with reinforcement learning. <i>PLoS Computational Biology</i> , 2018, 14, e1006176.	3.2	23
20	Variational encoding of complex dynamics. <i>Physical Review E</i> , 2018, 97, 062412.	2.1	119
21	Towards simple kinetic models of functional dynamics for a kinase subfamily. <i>Nature Chemistry</i> , 2018, 10, 903-909.	13.6	61
22	Computer Simulations Predict High Structural Heterogeneity of Functional State of NMDA Receptors. <i>Biophysical Journal</i> , 2018, 115, 841-852.	0.5	7
23	Communication: Adaptive boundaries in multiscale simulations. <i>Journal of Chemical Physics</i> , 2018, 148, 141104.	3.0	10
24	Engineering a Single-Agent Cytokine/Antibody Fusion That Selectively Expands Regulatory T Cells for Autoimmune Disease Therapy. <i>Journal of Immunology</i> , 2018, 201, 2094-2106.	0.8	58
25	MSMBuilder: Statistical Models for Biomolecular Dynamics. <i>Biophysical Journal</i> , 2017, 112, 10-15.	0.5	228
26	Identification of simple reaction coordinates from complex dynamics. <i>Journal of Chemical Physics</i> , 2017, 146, 044109.	3.0	73
27	Ward Clustering Improves Cross-Validated Markov State Models of Protein Folding. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 963-967.	5.3	38
28	Efficient gaussian density formulation of volume and surface areas of macromolecules on graphical processing units. <i>Journal of Computational Chemistry</i> , 2017, 38, 740-752.	3.3	11
29	Markov modeling reveals novel intracellular modulation of the human TREK-2 selectivity filter. <i>Scientific Reports</i> , 2017, 7, 632.	3.3	15
30	Quercitrin and quercetin 3- β -D-glucoside as chemical chaperones for the A4V SOD1 ALS-causing mutant. <i>Protein Engineering, Design and Selection</i> , 2017, 30, 431-440.	2.1	33
31	Low Data Drug Discovery with One-Shot Learning. <i>ACS Central Science</i> , 2017, 3, 283-293.	11.3	511
32	Atomistic structural ensemble refinement reveals non-native structure stabilizes a sub-millisecond folding intermediate of CheY. <i>Scientific Reports</i> , 2017, 7, 44116.	3.3	10
33	tICA-Metadynamics: Accelerating Metadynamics by Using Kinetically Selected Collective Variables. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2440-2447.	5.3	142
34	Computationally Discovered Potentiating Role of Glycans on NMDA Receptors. <i>Scientific Reports</i> , 2017, 7, 44578.	3.3	25
35	Building a More Predictive Protein Force Field: A Systematic and Reproducible Route to AMBER-FB15. <i>Journal of Physical Chemistry B</i> , 2017, 121, 4023-4039.	2.6	192
36	Solution-Phase Conformation and Dynamics of Conjugated Isoindigo-Based Donor-Acceptor Polymer Single Chains. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 5479-5486.	4.6	24

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37	Simulated Dynamics of Glycans on Ligand-Binding Domain of NMDA Receptors Reveals Strong Dynamic Coupling between Glycans and Protein Core. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5496-5505.	5.3	17
38	Modeling the mechanism of CLN025 beta-hairpin formation. <i>Journal of Chemical Physics</i> , 2017, 147, 104107.	3.0	34
39	Retrosynthetic Reaction Prediction Using Neural Sequence-to-Sequence Models. <i>ACS Central Science</i> , 2017, 3, 1103-1113.	11.3	308
40	An information theoretic framework reveals a tunable allosteric network in group II chaperonins. <i>Nature Structural and Molecular Biology</i> , 2017, 24, 726-733.	8.2	14
41	Millisecond dynamics of BTK reveal kinome-wide conformational plasticity within the apo kinase domain. <i>Scientific Reports</i> , 2017, 7, 15604.	3.3	43
42	Note: MSM lag time cannot be used for variational model selection. <i>Journal of Chemical Physics</i> , 2017, 147, 176101.	3.0	16
43	Is Multitask Deep Learning Practical for Pharma?. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 2068-2076.	5.4	191
44	OpenMM 7: Rapid development of high performance algorithms for molecular dynamics. <i>PLoS Computational Biology</i> , 2017, 13, e1005659.	3.2	1,561
45	Discovery of novel brain permeable and G protein-biased beta-1 adrenergic receptor partial agonists for the treatment of neurocognitive disorders. <i>PLoS ONE</i> , 2017, 12, e0180319.	2.5	22
46	Finding Our Way in the Dark Proteome. <i>Journal of the American Chemical Society</i> , 2016, 138, 9730-9742.	13.7	111
47	Conformational heterogeneity of the calmodulin binding interface. <i>Nature Communications</i> , 2016, 7, 10910.	12.8	49
48	Optimized parameter selection reveals trends in Markov state models for protein folding. <i>Journal of Chemical Physics</i> , 2016, 145, 194103.	3.0	61
49	Tungstate as a Transition State Analog for Catalysis by Alkaline Phosphatase. <i>Journal of Molecular Biology</i> , 2016, 428, 2758-2768.	4.2	22
50	Markov State Models and tICA Reveal a Nonnative Folding Nucleus in Simulations of NuG2. <i>Biophysical Journal</i> , 2016, 110, 1716-1719.	0.5	34
51	Transition path theory analysis of c-Src kinase activation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, 9193-9198.	7.1	67
52	Advanced Potential Energy Surfaces for Molecular Simulation. <i>Journal of Physical Chemistry B</i> , 2016, 120, 9811-9832.	2.6	77
53	CHARMM-GUI Input Generator for NAMD, GROMACS, AMBER, OpenMM, and CHARMM/OpenMM Simulations Using the CHARMM36 Additive Force Field. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 405-413.	5.3	2,567
54	Discovery of a regioselectivity switch in nitrating P450s guided by molecular dynamics simulations and Markov models. <i>Nature Chemistry</i> , 2016, 8, 419-425.	13.6	107

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55	Identification of significantly mutated regions across cancer types highlights a rich landscape of functional molecular alterations. <i>Nature Genetics</i> , 2016, 48, 117-125.	21.4	80
56	Efficient maximum likelihood parameterization of continuous-time Markov processes. <i>Journal of Chemical Physics</i> , 2015, 143, 034109.	3.0	23
57	Modeling Molecular Kinetics with tICA and the Kernel Trick. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 600-608.	5.3	115
58	Conserve Water: A Method for the Analysis of Solvent in Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1094-1101.	5.3	14
59	Revised Parameters for the AMOEBA Polarizable Atomic Multipole Water Model. <i>Journal of Physical Chemistry B</i> , 2015, 119, 9423-9437.	2.6	183
60	Heat dissipation guides activation in signaling proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 10377-10382.	7.1	27
61	Cloud computing approaches for prediction of ligand binding poses and pathways. <i>Scientific Reports</i> , 2015, 5, 7918.	3.3	54
62	Potential-Based Dynamical Reweighting for Markov State Models of Protein Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2412-2420.	5.3	5
63	A network of molecular switches controls the activation of the two-component response regulator NtrC. <i>Nature Communications</i> , 2015, 6, 7283.	12.8	40
64	Entropy-production-driven oscillators in simple nonequilibrium networks. <i>Physical Review E</i> , 2015, 91, 032136.	2.1	4
65	Elucidating Ligand-Modulated Conformational Landscape of GPCRs Using Cloud-Computing Approaches. <i>Methods in Enzymology</i> , 2015, 557, 551-572.	1.0	15
66	Percolation-like phase transitions in network models of protein dynamics. <i>Journal of Chemical Physics</i> , 2015, 142, 215105.	3.0	8
67	United polarizable multipole water model for molecular mechanics simulation. <i>Journal of Chemical Physics</i> , 2015, 143, 014504.	3.0	36
68	MDTraj: A Modern Open Library for the Analysis of Molecular Dynamics Trajectories. <i>Biophysical Journal</i> , 2015, 109, 1528-1532.	0.5	1,576
69	Variational cross-validation of slow dynamical modes in molecular kinetics. <i>Journal of Chemical Physics</i> , 2015, 142, 124105.	3.0	173
70	The Dynamic Conformational Cycle of the Group I Chaperonin C-Termini Revealed via Molecular Dynamics Simulation. <i>PLoS ONE</i> , 2015, 10, e0117724.	2.5	8
71	Understanding Protein Folding Yields Important Insights into Protein Conformational Change: New Insights into Kinases and GPCRs. <i>FASEB Journal</i> , 2015, 29, 356.1.	0.5	0
72	Automatic Selection of Order Parameters in the Analysis of Large Scale Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5217-5223.	5.3	23

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73	Bayesian Energy Landscape Tilting: Towards Concordant Models of Molecular Ensembles. Biophysical Journal, 2014, 106, 1381-1390.	0.5	58
74	A Molecular Interpretation of 2D IR Protein Folding Experiments with Markov State Models. Biophysical Journal, 2014, 106, 1359-1370.	0.5	48
75	Activation pathway of Src kinase reveals intermediate states as targets for drug design. Nature Communications, 2014, 5, 3397.	12.8	300
76	Cloud-based simulations on Google Exacycle reveal ligand modulation of GPCR activation pathways. Nature Chemistry, 2014, 6, 15-21.	13.6	388
77	Discovering chemistry with an ab initio nanoreactor. Nature Chemistry, 2014, 6, 1044-1048.	13.6	286
78	Dynamical Phase Transitions Reveal Amyloid-like States on Protein Folding Landscapes. Biophysical Journal, 2014, 107, 974-982.	0.5	24
79	Complex Pathways in Folding of Protein G Explored by Simulation and Experiment. Biophysical Journal, 2014, 107, 947-955.	0.5	41
80	Building Force Fields: An Automatic, Systematic, and Reproducible Approach. Journal of Physical Chemistry Letters, 2014, 5, 1885-1891.	4.6	400
81	Long Timestep Molecular Dynamics on the Graphical Processing Unit. Journal of Chemical Theory and Computation, 2013, 9, 3267-3281.	5.3	20
82	K-Means for Parallel Architectures Using All-Prefix-Sum Sorting and Updating Steps. IEEE Transactions on Parallel and Distributed Systems, 2013, 24, 1602-1612.	5.6	23
83	Accelerated Molecular Dynamics Simulations with the AMOEBA Polarizable Force Field on Graphics Processing Units. Journal of Chemical Theory and Computation, 2013, 9, 4684-4691.	5.3	39
84	To milliseconds and beyond: challenges in the simulation of protein folding. Current Opinion in Structural Biology, 2013, 23, 58-65.	5.7	331
85	Improvements in Markov State Model Construction Reveal Many Non-Native Interactions in the Folding of NTL9. Journal of Chemical Theory and Computation, 2013, 9, 2000-2009.	5.3	506
86	Learning Kinetic Distance Metrics for Markov State Models of Protein Conformational Dynamics. Journal of Chemical Theory and Computation, 2013, 9, 2900-2906.	5.3	43
87	Finite domain simulations with adaptive boundaries: Accurate potentials and nonequilibrium movesets. Journal of Chemical Physics, 2013, 139, 234114.	3.0	12
88	Mechanistic and structural insight into the functional dichotomy between IL-2 and IL-15. Nature Immunology, 2012, 13, 1187-1195.	14.5	206
89	Exploiting a natural conformational switch to engineer an interleukin-2 "superkine". Nature, 2012, 484, 529-533.	27.8	438
90	Chaperonins: The Machines Which Fold Proteins. , 2011, , 87-98.		0

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91	MSMBuilder2: Modeling Conformational Dynamics on the Picosecond to Millisecond Scale. Journal of Chemical Theory and Computation, 2011, 7, 3412-3419.	5.3	381
92	(Compressed) sensing and sensibility. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 14713-14714.	7.1	3
93	OpenMM: A Hardware-Independent Framework for Molecular Simulations. Computing in Science and Engineering, 2010, 12, 34-39.	1.2	195
94	Hard Data on Soft Errors: A Large-Scale Assessment of Real-World Error Rates in GPGPU. , 2010, , .		74
95	Everything you wanted to know about Markov State Models but were afraid to ask. Methods, 2010, 52, 99-105.	3.8	591
96	Simple Theory of Protein Folding Kinetics. Physical Review Letters, 2010, 105, 198101.	7.8	23
97	Thalweg: A framework for programming 1,000 machines with 1,000 cores. , 2009, , .		0
98	Folding@home: Lessons from eight years of volunteer distributed computing. , 2009, , .		136
99	Storage@home: Petascale Distributed Storage. , 2007, , .		18
100	PREDICTING STRUCTURE AND DYNAMICS OF LOOSELY-ORDERED PROTEIN COMPLEXES: INFLUENZA HEMAGGLUTININ FUSION PEPTIDE. , 2006, , .		3
101	Control of membrane fusion mechanism by lipid composition: predictions from ensemble molecular dynamics. PLoS Computational Biology, 2005, preprint, e220.	3.2	2
102	Extremely precise free energy calculations of amino acid side chain analogs: Comparison of common molecular mechanics force fields for proteins. Journal of Chemical Physics, 2003, 119, 5740-5761.	3.0	611
103	Atomistic protein folding simulations on the submillisecond time scale using worldwide distributed computing. Biopolymers, 2003, 68, 91-109.	2.4	346
104	Meeting halfway on the bridge between protein folding theory and experiment. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 3555-3556.	7.1	22
105	A New Twist on the Helix-Coil Transition: A Non-Biological Helix with Protein-Like Intermediates and Traps. Journal of Physical Chemistry B, 2001, 105, 482-485.	2.6	28
106	COMPUTING: Screen Savers of the World Unite!. Science, 2000, 290, 1903-1904.	12.6	491