Vijay S Pande

List of Publications by Year
in descending order

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106 papers	17,923 citations	66250 44 h-index	37326 100 g-index
110 all docs	110 docs citations	110 times ranked	19683 citing authors

#	Article	IF	Citations
1	Computational IR Spectroscopy of Insulin Dimer Structure and Conformational Heterogeneity. Journal of Physical Chemistry B, 2021, 125, 4620-4633.	1.2	14
2	A Targeted Computational Screen of the SWEETLEAD Database Reveals FDA-Approved Compounds with Anti-Dengue Viral Activity. MBio, 2020, 11, .	1.8	6
3	Dynamical model of the CLC-2 ion channel reveals conformational changes associated with selectivity-filter gating. PLoS Computational Biology, 2020, 16, e1007530.	1.5	9
4	Improvement in ADMET Prediction with Multitask Deep Featurization. Journal of Medicinal Chemistry, 2020, 63, 8835-8848.	2.9	110
5	A modular DNA scaffold to study proteinâ€“protein interactions at single-molecule resolution. Nature Nanotechnology, 2019, 14, 988-993.	15.6	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 (*lf*1) receptor selective ligands. European Journal of Medicinal Chemistry, 2019, 164, 241-251.	2.6	5
7	Intradomain Interactions in an NMDA Receptor Fragment Mediate N-Glycan Processing and Conformational Sampling. Structure, 2019, 27, 55-65.e3.	1.6	9
8	Theoretical restrictions on longest implicit time scales in Markov state models of biomolecular dynamics. Journal of Chemical Physics, 2018, 148, 044111.	1.2	4
9	A Minimum Variance Clustering Approach Produces Robust and Interpretable Coarse-Grained Models. Journal of Chemical Theory and Computation, 2018, 14, 1071-1082.	2.3	16
10	Markov State Models: From an Art to a Science. Journal of the American Chemical Society, 2018, 140, 2386-2396.	6.6	573
11	REDOR NMR Reveals Multiple Conformers for a Protein Kinase C Ligand in a Membrane Environment. ACS Central Science, 2018, 4, 89-96.	5.3	28
12	MoleculeNet: a benchmark for molecular machine learning. Chemical Science, 2018, 9, 513-530.	3.7	1,261
13	Transfer Learning from Markov Models Leads to Efficient Sampling of Related Systems. Journal of Physical Chemistry B, 2018, 122, 5291-5299.	1.2	14
14	Perspective: Computational chemistry software and its advancement as illustrated through three grand challenge cases for molecular science. Journal of Chemical Physics, 2018, 149, 180901.	1.2	72
15	Note: Variational encoding of protein dynamics benefits from maximizing latent autocorrelation. Journal of Chemical Physics, 2018, 149, 216101.	1.2	7
16	Bayesian analysis of isothermal titration calorimetry for binding thermodynamics. PLoS ONE, 2018, 13, e0203224.	1.1	24
17	PotentialNet for Molecular Property Prediction. ACS Central Science, 2018, 4, 1520-1530.	5.3	278
18	Automated design of collective variables using supervised machine learning. Journal of Chemical Physics, 2018, 149, 094106.	1.2	98

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19	Solving the RNA design problem with reinforcement learning. PLoS Computational Biology, 2018, 14, e1006176.	1.5	23
20	Variational encoding of complex dynamics. Physical Review E, 2018, 97, 062412.	0.8	119
21	Towards simple kinetic models of functional dynamics for a kinase subfamily. Nature Chemistry, 2018, 10, 903-909.	6.6	61
22	Computer Simulations Predict High Structural Heterogeneity of Functional State of NMDA Receptors. Biophysical Journal, 2018, 115, 841-852.	0.2	7
23	Communication: Adaptive boundaries in multiscale simulations. Journal of Chemical Physics, 2018, 148, 141104.	1.2	10
24	Engineering a Single-Agent Cytokine/Antibody Fusion That Selectively Expands Regulatory T Cells for Autoimmune Disease Therapy. Journal of Immunology, 2018, 201, 2094-2106.	0.4	58
25	MSMBuilder: Statistical Models for Biomolecular Dynamics. Biophysical Journal, 2017, 112, 10-15.	0.2	228
26	Identification of simple reaction coordinates from complex dynamics. Journal of Chemical Physics, 2017, 146, 044109.	1.2	73
27	Ward Clustering Improves Cross-Validated Markov State Models of Protein Folding. Journal of Chemical Theory and Computation, 2017, 13, 963-967.	2.3	38
28	Efficient gaussian density formulation of volume and surface areas of macromolecules on graphical processing units. Journal of Computational Chemistry, 2017, 38, 740-752.	1.5	11
29	Markov modeling reveals novel intracellular modulation of the human TREK-2 selectivity filter. Scientific Reports, 2017, 7, 632.	1.6	15
30	Quercitrin and quercetin 3-Î²-d-glucoside as chemical chaperones for the A4V SOD1 ALS-causing mutant. Protein Engineering, Design and Selection, 2017, 30, 431-440.	1.0	33
31	Low Data Drug Discovery with One-Shot Learning. ACS Central Science, 2017, 3, 283-293.	5.3	511
32	Atomistic structural ensemble refinement reveals non-native structure stabilizes a sub-millisecond folding intermediate of CheY. Scientific Reports, 2017, 7, 44116.	1.6	10
33	tICA-Metadynamics: Accelerating Metadynamics by Using Kinetically Selected Collective Variables. Journal of Chemical Theory and Computation, 2017, 13, 2440-2447.	2.3	142
34	Computationally Discovered Potentiating Role of Glycans on NMDA Receptors. Scientific Reports, 2017, 7, 44578.	1.6	25
35	Building a More Predictive Protein Force Field: A Systematic and Reproducible Route to AMBER-FB15. Journal of Physical Chemistry B, 2017, 121, 4023-4039.	1.2	192
36	Solution-Phase Conformation and Dynamics of Conjugated Isoindigo-Based Donorâ€“Acceptor Polymer Single Chains. Journal of Physical Chemistry Letters, 2017, 8, 5479-5486.	2.1	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. Journal of Chemical Theory and Computation, 2017, 13, 5496-5505.	2.3	17
38	Modeling the mechanism of CLN025 beta-hairpin formation. Journal of Chemical Physics, 2017, 147, 104107.	1.2	34
39	Retrosynthetic Reaction Prediction Using Neural Sequence-to-Sequence Models. ACS Central Science, 2017, 3, 1103-1113.	5.3	308
40	An information theoretic framework reveals a tunable allosteric network in group II chaperonins. Nature Structural and Molecular Biology, 2017, 24, 726-733.	3.6	14
41	Millisecond dynamics of BTK reveal kinome-wide conformational plasticity within the apo kinase domain. Scientific Reports, 2017, 7, 15604.	1.6	43
42	Note: MSM lag time cannot be used for variational model selection. Journal of Chemical Physics, 2017, 147, 176101.	1.2	16
43	Is Multitask Deep Learning Practical for Pharma?. Journal of Chemical Information and Modeling, 2017, 57, 2068-2076.	2.5	191
44	OpenMM 7: Rapid development of high performance algorithms for molecular dynamics. PLoS Computational Biology, 2017, 13, e1005659.	1.5	1,561
45	Discovery of novel brain permeable and G protein-biased beta-1 adrenergic receptor partial agonists for the treatment of neurocognitive disorders. PLoS ONE, 2017, 12, e0180319.	1.1	22
46	Finding Our Way in the Dark Proteome. Journal of the American Chemical Society, 2016, 138, 9730-9742.	6.6	111
47	Conformational heterogeneity of the calmodulin binding interface. Nature Communications, 2016, 7, 10910.	5.8	49
48	Optimized parameter selection reveals trends in Markov state models for protein folding. Journal of Chemical Physics, 2016, 145, 194103.	1.2	61
49	Tungstate as a Transition State Analog for Catalysis by Alkaline Phosphatase. Journal of Molecular Biology, 2016, 428, 2758-2768.	2.0	22
50	Markov State Models and tICA Reveal a Nonnative Folding Nucleus in Simulations of NuG2. Biophysical Journal, 2016, 110, 1716-1719.	0.2	34
51	Transition path theory analysis of c-Src kinase activation. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 9193-9198.	3.3	67
52	Advanced Potential Energy Surfaces for Molecular Simulation. Journal of Physical Chemistry B, 2016, 120, 9811-9832.	1.2	77
53	CHARMM-GUI Input Generator for NAMD, GROMACS, AMBER, OpenMM, and CHARMM/OpenMM Simulations Using the CHARMM36 Additive Force Field. Journal of Chemical Theory and Computation, 2016, 12, 405-413.	2.3	2,567
54	Discovery of a regioselectivity switch in nitrating P450s guided by molecular dynamics simulations and Markov models. Nature Chemistry, 2016, 8, 419-425.	6.6	107

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55	Identification of significantly mutated regions across cancer types highlights a rich landscape of functional molecular alterations. Nature Genetics, 2016, 48, 117-125.	9.4	80
56	Efficient maximum likelihood parameterization of continuous-time Markov processes. Journal of Chemical Physics, 2015, 143, 034109.	1.2	23
57	Modeling Molecular Kinetics with tICA and the Kernel Trick. Journal of Chemical Theory and Computation, 2015, 11, 600-608.	2.3	115
58	Conserve Water: A Method for the Analysis of Solvent in Molecular Dynamics. Journal of Chemical Theory and Computation, 2015, 11, 1094-1101.	2.3	14
59	Revised Parameters for the AMOEBA Polarizable Atomic Multipole Water Model. Journal of Physical Chemistry B, 2015, 119, 9423-9437.	1.2	183
60	Heat dissipation guides activation in signaling proteins. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 10377-10382.	3.3	27
61	Cloud computing approaches for prediction of ligand binding poses and pathways. Scientific Reports, 2015, 5, 7918.	1.6	54
62	Potential-Based Dynamical Reweighting for Markov State Models of Protein Dynamics. Journal of Chemical Theory and Computation, 2015, 11, 2412-2420.	2.3	5
63	A network of molecular switches controls the activation of the two-component response regulator NtrC. Nature Communications, 2015, 6, 7283.	5.8	40
64	Entropy-production-driven oscillators in simple nonequilibrium networks. Physical Review E, 2015, 91, 032136.	0.8	4
65	Elucidating Ligand-Modulated Conformational Landscape of GPCRs Using Cloud-Computing Approaches. Methods in Enzymology, 2015, 557, 551-572.	0.4	15
66	Percolation-like phase transitions in network models of protein dynamics. Journal of Chemical Physics, 2015, 142, 215105.	1.2	8
67	United polarizable multipole water model for molecular mechanics simulation. Journal of Chemical Physics, 2015, 143, 014504.	1.2	36
68	MDTraj: A Modern Open Library for the Analysis of Molecular Dynamics Trajectories. Biophysical Journal, 2015, 109, 1528-1532.	0.2	1,576
69	Variational cross-validation of slow dynamical modes in molecular kinetics. Journal of Chemical Physics, 2015, 142, 124105.	1.2	173
70	The Dynamic Conformational Cycle of the Group I Chaperonin C-Termini Revealed via Molecular Dynamics Simulation. PLoS ONE, 2015, 10, e0117724.	1.1	8
71	Understanding Protein Folding Yields Important Insights into Protein Conformational Change: New Insights into Kinases and GPCRs. FASEB Journal, 2015, 29, 356.1.	0.2	0
72	Automatic Selection of Order Parameters in the Analysis of Large Scale Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2014, 10, 5217-5223.	2.3	23

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73	Bayesian Energy Landscape Tilting: Towards Concordant Models of Molecular Ensembles. Biophysical Journal, 2014, 106, 1381-1390.	0.2	58
74	A Molecular Interpretation of 2D IR Protein Folding Experiments with Markov State Models. Biophysical Journal, 2014, 106, 1359-1370.	0.2	48
75	Activation pathway of Src kinase reveals intermediate states as targets for drug design. Nature Communications, 2014, 5, 3397.	5.8	300
76	Cloud-based simulations on Google Exacycle reveal ligand modulation of GPCR activation pathways. Nature Chemistry, 2014, 6, 15-21.	6.6	388
77	Discovering chemistry with an ab initio nanoreactor. Nature Chemistry, 2014, 6, 1044-1048.	6.6	286
78	Dynamical Phase Transitions Reveal Amyloid-like States on Protein Folding Landscapes. Biophysical Journal, 2014, 107, 974-982.	0.2	24
79	Complex Pathways in Folding of Protein G Explored by Simulation and Experiment. Biophysical Journal, 2014, 107, 947-955.	0.2	41
80	Building Force Fields: An Automatic, Systematic, and Reproducible Approach. Journal of Physical Chemistry Letters, 2014, 5, 1885-1891.	2.1	400
81	Long Timestep Molecular Dynamics on the Graphical Processing Unit. Journal of Chemical Theory and Computation, 2013, 9, 3267-3281.	2.3	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.	4.0	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.	2.3	39
84	To milliseconds and beyond: challenges in the simulation of protein folding. Current Opinion in Structural Biology, 2013, 23, 58-65.	2.6	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.	2.3	506
86	Learning Kinetic Distance Metrics for Markov State Models of Protein Conformational Dynamics. Journal of Chemical Theory and Computation, 2013, 9, 2900-2906.	2.3	43
87	Finite domain simulations with adaptive boundaries: Accurate potentials and nonequilibrium movesets. Journal of Chemical Physics, 2013, 139, 234114.	1.2	12
88	Mechanistic and structural insight into the functional dichotomy between IL-2 and IL-15. Nature Immunology, 2012, 13, 1187-1195.	7.0	206
89	Exploiting a natural conformational switch to engineer an interleukin-2 â€˜superkineâ€™. Nature, 2012, 484, 529-533.	13.7	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.	2.3	381
92	(Compressed) sensing and sensibility. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 14713-14714.	3.3	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.	1.9	591
96	Simple Theory of Protein Folding Kinetics. Physical Review Letters, 2010, 105, 198101.	2.9	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.	1.5	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.	1.2	611
103	Atomistic protein folding simulations on the submillisecond time scale using worldwide distributed computing. Biopolymers, 2003, 68, 91-109.	1.2	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.	3.3	22
105	A New Twist on the Helix-Coil Transition:Â A Non-Biological Helix with Protein-Like Intermediates and Traps. Journal of Physical Chemistry B, 2001, 105, 482-485.	1.2	28
106	COMPUTING: Screen Savers of the World Unite!. Science, 2000, 290, 1903-1904.	6.0	491