Cecilia Clementi

List of Publications by Year
in descending order

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85	7,191	71102	60623
papers	citations	41 h-index	81 g-index

88	88	88	4937
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Topological and energetic factors: what determines the structural details of the transition state ensemble and â€œen-routeâ€•intermediates for protein folding? an investigation for small globular proteins. Journal of Molecular Biology, 2000, 298, 937-953.	4.2	1,136
2	Machine Learning for Molecular Simulation. Annual Review of Physical Chemistry, 2020, 71, 361-390.	10.8	456
3	Machine Learning of Coarse-Grained Molecular Dynamics Force Fields. ACS Central Science, 2019, 5, 755-767.	11.3	306
4	Coarse-grained models of protein folding: toy models or predictive tools?. Current Opinion in Structural Biology, 2008, 18, 10-15.	5.7	294
5	Low-dimensional, free-energy landscapes of protein-folding reactions by nonlinear dimensionality reduction. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 9885-9890.	7.1	293
6	AWSEM-MD: Protein Structure Prediction Using Coarse-Grained Physical Potentials and Bioinformatically Based Local Structure Biasing. Journal of Physical Chemistry B, 2012, 116, 8494-8503.	2.6	276
7	Determination of reaction coordinates via locally scaled diffusion map. Journal of Chemical Physics, 2011, 134, 124116.	3.0	212
8	Quantifying the Roughness on the Free Energy Landscape:Â Entropic Bottlenecks and Protein Folding Rates. Journal of the American Chemical Society, 2004, 126, 8426-8432.	13.7	211
9	Unsupervised Learning Methods for Molecular Simulation Data. Chemical Reviews, 2021, 121, 9722-9758.	47.7	182
10	Discovering Mountain Passes via Torchlight: Methods for the Definition of Reaction Coordinates and Pathways in Complex Macromolecular Reactions. Annual Review of Physical Chemistry, 2013, 64, 295-316.	10.8	177
11	Kinetic Distance and Kinetic Maps from Molecular Dynamics Simulation. Journal of Chemical Theory and Computation, 2015, 11, 5002-5011.	5.3	173
12	Interplay Among Tertiary Contacts, Secondary Structure Formation and Side-chain Packing in the Protein Folding Mechanism: All-atom Representation Study of Protein L. Journal of Molecular Biology, 2003, 326, 933-954.	4.2	167
13	The effects of nonnative interactions on protein folding rates: Theory and simulation. Protein Science, 2004, 13, 1750-1766.	7.6	158
14	Sparse learning of stochastic dynamical equations. Journal of Chemical Physics, 2018, 148, 241723.	3.0	130
15	Data-driven approximation of the Koopman generator: Model reduction, system identification, and control. Physica D: Nonlinear Phenomena, 2020, 406, 132416.	2.8	128
16	Jaggedâ€“Delta asymmetry in Notch signaling can give rise to a Sender/Receiver hybrid phenotype. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E402-9.	7.1	127
17	Collective variables for the study of long-time kinetics from molecular trajectories: theory and methods. Current Opinion in Structural Biology, 2017, 43, 141-147.	5.7	116
18	Machine learning for protein folding and dynamics. Current Opinion in Structural Biology, 2020, 60, 77-84.	5.7	116

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19	From coarse-grain to all-atom: Toward multiscale analysis of protein landscapes. Proteins: Structure, Function and Bioinformatics, 2007, 68, 646-661.	2.6	111
20	Coarse graining molecular dynamics with graph neural networks. Journal of Chemical Physics, 2020, 153, 194101.	3.0	103
21	TorchMD: A Deep Learning Framework for Molecular Simulations. Journal of Chemical Theory and Computation, 2021, 17, 2355-2363.	5.3	101
22	Balancing energy and entropy: A minimalist model for the characterization of protein folding landscapes. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 10141-10146.	7.1	96
23	Fast recovery of free energy landscapes via diffusion-map-directed molecular dynamics. Physical Chemistry Chemical Physics, 2014, 16, 19181-19191.	2.8	96
24	Combining experimental and simulation data of molecular processes via augmented Markov models. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 8265-8270.	7.1	93
25	Prediction of folding mechanism for circular-permuted proteins. Journal of Molecular Biology, 2001, 311, 879-890.	4.2	86
26	Adaptive resolution simulation of liquid water. Journal of Physics Condensed Matter, 2007, 19, 292201.	1.8	85
27	Perspective: Computational chemistry software and its advancement as illustrated through three grand challenge cases for molecular science. Journal of Chemical Physics, 2018, 149, 180901.	3.0	72
28	Modeling protein conformational ensembles: From missing loops to equilibrium fluctuations. Proteins: Structure, Function and Bioinformatics, 2006, 65, 164-179.	2.6	71
29	Rapid Exploration of Configuration Space with Diffusion-Map-Directed Molecular Dynamics. Journal of Physical Chemistry B, 2013, 117, 12769-12776.	2.6	71
30	Modeling diffusive dynamics in adaptive resolution simulation of liquid water. Journal of Chemical Physics, 2008, 128, 024503.	3.0	66
31	Optimal Combination of Theory and Experiment for the Characterization of the Protein Folding Landscape of S6: How Far Can a Minimalist Model Go?. Journal of Molecular Biology, 2004, 343, 235-248.	4.2	64
32	Multiscale characterization of protein conformational ensembles. Proteins: Structure, Function and Bioinformatics, 2009, 76, 837-851.	2.6	63
33	Minimalist Protein Model as a Diagnostic Tool for Misfolding and Aggregation. Journal of Molecular Biology, 2006, 363, 297-308.	4.2	56
34	Application of nonlinear dimensionality reduction to characterize the conformational landscape of small peptides. Proteins: Structure, Function and Bioinformatics, 2010, 78, 223-235.	2.6	55
35	Investigating Molecular Kinetics by Variationally Optimized Diffusion Maps. Journal of Chemical Theory and Computation, 2015, 11, 5947-5960.	5.3	54
36	Markov state models from short non-equilibrium simulationsâ€"Analysis and correction of estimation bias. Journal of Chemical Physics, 2017, 146, .	3.0	51

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37	Folding, Design, and Determination of Interaction Potentials Using Off-Lattice Dynamics of Model Heteropolymers. Physical Review Letters, 1998, 81, 3287-3290.	7.8	50
38	Characterization of the folding landscape of monomeric lactose repressor: Quantitative comparison of theory and experiment. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 14569-14574.	7.1	49
39	Quantitative comparison of adaptive sampling methods for protein dynamics. Journal of Chemical Physics, 2018, 149, 244119.	3.0	49
40	Commute Maps: Separating Slowly Mixing Molecular Configurations for Kinetic Modeling. Journal of Chemical Theory and Computation, 2016, 12, 5620-5630.	5.3	47
41	Polymer reversal rate calculated via locally scaled diffusion map. Journal of Chemical Physics, 2011, 134, 144109.	3.0	44
42	Fast and reliable analysis of molecular motion using proximity relations and dimensionality reduction. Proteins: Structure, Function and Bioinformatics, 2007, 67, 897-907.	2.6	41
43	Delineation of Folding Pathways of a Î²-Sheet Miniprotein. Journal of Physical Chemistry B, 2011, 115, 13065-13074.	2.6	41
44	A tripodal peptide ligand for asymmetric Rh(<scp>ii</scp>) catalysis highlights unique features of on-bead catalyst development. Chemical Science, 2014, 5, 1401-1407.	7.4	40
45	APE-Gen: A Fast Method for Generating Ensembles of Bound Peptide-MHC Conformations. Molecules, 2019, 24, 881.	3.8	40
46	Surveying biomolecular frustration at atomic resolution. Nature Communications, 2020, 11, 5944.	12.8	40
47	Ensemble learning of coarse-grained molecular dynamics force fields with a kernel approach. Journal of Chemical Physics, 2020, 152, 194106.	3.0	38
48	Machine learning meets chemical physics. Journal of Chemical Physics, 2021, 154, 160401.	3.0	37
49	On the Characterization of Protein Native State Ensembles. Biophysical Journal, 2007, 92, 1503-1511.	0.5	36
50	Introduction: Machine Learning at the Atomic Scale. Chemical Reviews, 2021, 121, 9719-9721.	47.7	36
51	Machine learning implicit solvation for molecular dynamics. Journal of Chemical Physics, 2021, 155, 084101.	3.0	35
52	Restriction versus guidance in protein structure prediction. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 15302-15307.	7.1	34
53	Learning Effective Molecular Models from Experimental Observables. Journal of Chemical Theory and Computation, 2018, 14, 3849-3858.	5.3	34
54	Graphene, other carbon nanomaterials and the immune system: toward nanoimmunity-by-design. JPhys Materials, 2020, 3, 034009.	4.2	29

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55	Multi-body effects in a coarse-grained protein force field. Journal of Chemical Physics, 2021, 154, 164113.	3.0	28
56	The experimental folding landscape of monomeric lactose repressor, a large two-domain protein, involves two kinetic intermediates. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 14563-14568.	7.1	27
57	Coarse-graining molecular systems by spectral matching. Journal of Chemical Physics, 2019, 151, 044116.	3.0	26
58	Rapid Calculation of Molecular Kinetics Using Compressed Sensing. Journal of Chemical Theory and Computation, 2018, 14, 2771-2783.	5.3	24
59	A Data-Driven Perspective on the Hierarchical Assembly of Molecular Structures. Journal of Chemical Theory and Computation, 2018, 14, 453-460.	5.3	23
60	Unfolding the fold of cyclic cysteineâ€rich peptides. Protein Science, 2008, 17, 482-493.	7.6	22
61	Markov state modeling reveals alternative unbinding pathways for peptideâ€“MHC complexes. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 30610-30618.	7.1	22
62	Size and topology modulate the effects of frustration in protein folding. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 9234-9239.	7.1	21
63	Folding Lennard-Jones proteins by a contact potential. , 1999, 37, 544-553.		20
64	Molecular recognition of DNA by ligands: Roughness and complexity of the free energy profile. Journal of Chemical Physics, 2013, 139, 145102.	3.0	20
65	Rapid assessment of T-cell receptor specificity of the immune repertoire. Nature Computational Science, 2021, 1, 362-373.	8.0	20
66	Large-Scale Structure-Based Prediction of Stable Peptide Binding to Class I HLAs Using Random Forests. Frontiers in Immunology, 2020, 11, 1583.	4.8	19
67	Sampling Conformation Space to Model Equilibrium Fluctuations in Proteins. Algorithmica, 2007, 48, 303-327.	1.3	17
68	Mapping folding energy landscapes with theory and experiment. Archives of Biochemistry and Biophysics, 2008, 469, 29-33.	3.0	17
69	Nanoscale coupling of endocytic pit growth and stability. Science Advances, 2019, 5, eaax5775.	10.3	17
70	ExTASY: Scalable and flexible coupling of MD simulations and advanced sampling techniques. , 2016, , .		15
71	Localizing Frustration in Proteins Using All-Atom Energy Functions. Journal of Physical Chemistry B, 2019, 123, 4497-4504.	2.6	14
72	Extensible and Scalable Adaptive Sampling on Supercomputers. Journal of Chemical Theory and Computation, 2020, 16, 7915-7925.	5.3	14

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73	A comparative analysis of clustering algorithms: O2 migration in truncated hemoglobin I from transition networks. Journal of Chemical Physics, 2015, 142, 025103.	3.0	10
74	Hamiltonian dynamics of homopolymer chain models. Physical Review E, 2006, 74, 041805.	2.1	7
75	Think Globally, Move Locally: Coarse Graining of Effective Free Energy Surfaces. Lecture Notes in Computational Science and Engineering, 2011, , 113-131.	0.3	5
76	Multiscale Approach to the Determination of the Photoactive Yellow Protein Signaling State Ensemble. PLoS Computational Biology, 2014, 10, e1003797.	3.2	5
77	Spectral Properties of Effective Dynamics from Conditional Expectations. Entropy, 2021, 23, 134.	2.2	5
78	Porting Adaptive Ensemble Molecular Dynamics Workflows to the Summit Supercomputer. Lecture Notes in Computer Science, 2019, , 397-417.	1.3	5
79	Tensor-based computation of metastable and coherent sets. Physica D: Nonlinear Phenomena, 2021, 427, 133018.	2.8	4
80	Fast track to structural biology. Nature Chemistry, 2021, 13, 1032-1034.	13.6	3
81	The Effect of Electrostatic Interactions on the Folding Kinetics of a 3-Î±-Helical Bundle Protein Family. Journal of Physical Chemistry B, 2018, 122, 11800-11806.	2.6	2
82	Preface: Special Topic on Reaction Pathways. Journal of Chemical Physics, 2017, 147, 152401.	3.0	1
83	Characterization of Protein-Folding Landscapes by Coarse-Grained Models Incorporating Experimental Data. , 2008, , 157-170.		1
84	Simulations Reveal Multiple Intermediates in the Unzipping Mechanism of Neuronal SNARE Complex. Biophysical Journal, 2018, 115, 1470-1480.	0.5	0
85	Multiscale characterization of macromolecular dynamics. , 2013, , .		0