Alessandro Laio

List of Publications by Year
in descending order

154	21,295	34105 52	9589 142
papers	citations	h-index	g-index

160	160	160	16833
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Escaping free-energy minima. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 12562-12566.	7.1	4,527
2	Clustering by fast search and find of density peaks. Science, 2014, 344, 1492-1496.	12.6	3,709
3	Metadynamics: a method to simulate rare events and reconstruct the free energy in biophysics, chemistry and material science. Reports on Progress in Physics, 2008, 71, 126601.	20.1	1,334
4	Efficient Exploration of Reactive Potential Energy Surfaces Using Car-Parrinello Molecular Dynamics. Physical Review Letters, 2003, 90, 238302.	7.8	719
5	Predicting Crystal Structures: The Parrinello-Rahman Method Revisited. Physical Review Letters, 2003, 90, 075503.	7.8	591
6	A Hamiltonian electrostatic coupling scheme for hybrid Carâ€“Parrinello molecular dynamics simulations. Journal of Chemical Physics, 2002, 116, 6941-6947.	3.0	588
7	Amyloid Î² Protein and Alzheimerâ€™s Disease: When Computer Simulations Complement Experimental Studies. Chemical Reviews, 2015, 115, 3518-3563.	47.7	530
8	Efficient Reconstruction of Complex Free Energy Landscapes by Multiple Walkers Metadynamicsâ€. Journal of Physical Chemistry B, 2006, 110, 3533-3539.	2.6	511
9	A Bias-Exchange Approach to Protein Folding. Journal of Physical Chemistry B, 2007, 111, 4553-4559.	2.6	498
10	Free-Energy Landscape for Î² Hairpin Folding from Combined Parallel Tempering and Metadynamics. Journal of the American Chemical Society, 2006, 128, 13435-13441.	13.7	458
11	Assessing the Accuracy of Metadynamicsâ€. Journal of Physical Chemistry B, 2005, 109, 6714-6721.	2.6	446
12	Equilibrium Free Energies from Nonequilibrium Metadynamics. Physical Review Letters, 2006, 96, 090601.	7.8	355
13	Using metadynamics to explore complex free-energy landscapes. Nature Reviews Physics, 2020, 2, 200-212.	26.6	346
14	Physics of Iron at Earth's Core Conditions. Science, 2000, 287, 1027-1030.	12.6	341
15	Flexible Docking in Solution Using Metadynamics. Journal of the American Chemical Society, 2005, 127, 2600-2607.	13.7	266
16	A Kinetic Model of Trp-Cage Folding from Multiple Biased Molecular Dynamics Simulations. PLoS Computational Biology, 2009, 5, e1000452.	3.2	246
17	A Recipe for the Computation of the Free Energy Barrier and the Lowest Free Energy Path of Concerted Reactionsâ€. Journal of Physical Chemistry B, 2005, 109, 6676-6687.	2.6	243
18	An Efficient Real Space Multigrid QM/MM Electrostatic Coupling. Journal of Chemical Theory and Computation, 2005, 1, 1176-1184.	5.3	224

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19	Anisotropy of Earth's Dâ€³ layer and stacking faults in the MgSiO3 post-perovskite phase. Nature, 2005, 438, 1142-1144.	27.8	219
20	The Conformational Free Energy Landscape of Î²-<scp>d</scp>-Glucopyranose. Implications for Substrate Preactivation in Î²-Glucoside Hydrolases. Journal of the American Chemical Society, 2007, 129, 10686-10693.	13.7	196
21	D-RESP:â€‰ Dynamically Generated Electrostatic Potential Derived Charges from Quantum Mechanics/Molecular Mechanics Simulations. Journal of Physical Chemistry B, 2002, 106, 7300-7307.	2.6	187
22	Unsupervised Learning Methods for Molecular Simulation Data. Chemical Reviews, 2021, 121, 9722-9758.	47.7	182
23	A Collective Variable for the Efficient Exploration of Protein Beta-Sheet Structures: Application to SH3 and GB1. Journal of Chemical Theory and Computation, 2009, 5, 2197-2201.	5.3	153
24	An Efficient Linear-Scaling Electrostatic Coupling for Treating Periodic Boundary Conditions in QM/MM Simulations. Journal of Chemical Theory and Computation, 2006, 2, 1370-1378.	5.3	152
25	Reconstructing the Density of States by History-Dependent Metadynamics. Physical Review Letters, 2004, 92, 170601.	7.8	149
26	Estimating the intrinsic dimension of datasets by a minimal neighborhood information. Scientific Reports, 2017, 7, 12140.	3.3	135
27	Substrate Binding Mechanism of HIV-1 Protease from Explicit-Solvent Atomistic Simulations. Journal of the American Chemical Society, 2009, 131, 11811-11818.	13.7	132
28	Characterization of the free-energy landscapes of proteins by NMR-guided metadynamics. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 6817-6822.	7.1	122
29	The inverted free energy landscape of an intrinsically disordered peptide by simulations and experiments. Scientific Reports, 2015, 5, 15449.	3.3	118
30	QM/MM Car-Parrinello Molecular Dynamics Study of the Solvent Effects on the Ground State and on the First Excited Singlet State of Acetone in Water. ChemPhysChem, 2003, 4, 1177-1182.	2.1	110
31	Stability and Structure of Oligomers of the Alzheimer Peptide AÎ²16â€“22: From the Dimer to the 32-Mer. Biophysical Journal, 2006, 91, 3217-3229.	0.5	102
32	Dissociation Mechanism of Acetic Acid in Water. Journal of the American Chemical Society, 2006, 128, 11318-11319.	13.7	100
33	A Molecular Spring for Vision. Journal of the American Chemical Society, 2004, 126, 15328-15329.	13.7	98
34	Microscopic Mechanism of Antibiotics Translocation through a Porin. Biophysical Journal, 2004, 87, 58-64.	0.5	92
35	Simulation of structural phase transitions by metadynamics. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.8	92
36	METAGUI. A VMD interface for analyzing metadynamics and molecular dynamics simulations. Computer Physics Communications, 2012, 183, 203-211.	7.5	92

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37	Systematic Improvement of Classical Nucleation Theory. Physical Review Letters, 2012, 108, 225701.	7.8	88
38	Azulene-to-Naphthalene Rearrangement: The Car-Parrinello Metadynamics Method Explores Various Reaction Mechanisms. ChemPhysChem, 2004, 5, 1558-1568.	2.1	78
39	Automated Parametrization of Biomolecular Force Fields from Quantum Mechanics/Molecular Mechanics (QM/MM) Simulations through Force Matching. Journal of Chemical Theory and Computation, 2007, 3, 628-639.	5.3	78
40	Multidimensional View of Amyloid Fibril Nucleation in Atomistic Detail. Journal of the American Chemical Society, 2012, 134, 3886-3894.	13.7	78
41	A Minimum Free Energy Reaction Path for the E2 Reaction between Fluoro Ethane and a Fluoride Ion. Journal of the American Chemical Society, 2004, 126, 9492-9493.	13.7	73
42	Metadynamics convergence law in a multidimensional system. Physical Review E, 2010, 81, 055701.	2.1	73
43	Physical Origin of Selectivity in Ionic Channels of Biological Membranes. Biophysical Journal, 1999, 76, 129-148.	0.5	70
44	Influence of DNA Structure on the Reactivity of the Guanine Radical Cation. Chemistry - A European Journal, 2004, 10, 4846-4852.	3.3	70
45	Vacancy-vacancy interaction and oxygen diffusion in stabilized cubic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>ZrO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:ms first principles. Physical Review B, 2008, 78, .	3.2	69
46	â€œSite Bindingâ€•of Ca2+Ions to Polyacrylates in Water:Â A Molecular Dynamics Study of Coiling and Aggregation. Macromolecules, 2007, 40, 3437-3442.	4.8	67
47	Correlations among Hydrogen Bonds in Liquid Water. Physical Review Letters, 2004, 93, 087801.	7.8	65
48	A Novel Approach to the Investigation of Passive Molecular Permeation through Lipid Bilayers from Atomistic Simulations. Journal of Physical Chemistry B, 2012, 116, 8714-8721.	2.6	63
49	Hybrid QM/MM Car-Parrinello Simulations of Catalytic and Enzymatic Reactions. Chimia, 2002, 56, 13-19.	0.6	62
50	Exploring the Universe of Protein Structures beyond the Protein Data Bank. PLoS Computational Biology, 2010, 6, e1000957.	3.2	62
51	Atomistic Structure of Cobalt-Phosphate Nanoparticles for Catalytic Water Oxidation. ACS Nano, 2012, 6, 10497-10504.	14.6	62
52	Charge Localization in DNA Fibers. Physical Review Letters, 2005, 94, 158103.	7.8	53
53	Nucleation Process of a Fibril Precursor in the C-Terminal Segment of Amyloid-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î²</mml:mi></mml:math>. Physical Review Letters, 2013, 110, 168103.	7.8	53
54	Initial stages of salt crystal dissolution determined with ab initio molecular dynamics. Physical Chemistry Chemical Physics, 2011, 13, 13162.	2.8	51

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55	Predicting the Effect of a Point Mutation on a Protein Fold: The Villin and Advillin Headpieces and Their Pro62Ala Mutants. Journal of Molecular Biology, 2008, 375, 460-470.	4.2	49
56	A simple and efficient statistical potential for scoring ensembles of protein structures. Scientific Reports, 2012, 2, .	3.3	48
57	Reaction mechanism of caspases: Insights from QM/MM Car-Parrinello simulations. Proteins: Structure, Function and Bioinformatics, 2003, 52, 212-224.	2.6	47
58	Cytoskeletal actin networks in motile cells are critically self-organized systems synchronized by mechanical interactions. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 13978-13983.	7.1	44
59	Protein Folding and Ligand-Enzyme Binding from Bias-Exchange Metadynamics Simulations. Current Physical Chemistry, 2012, 2, 79-91.	0.2	44
60	Role of Enzyme Flexibility in Ligand Access and Egress to Active Site: Bias-Exchange Metadynamics Study of 1,3,7-Trimethyluric Acid in Cytochrome P450 3A4. Journal of Chemical Theory and Computation, 2016, 12, 2101-2109.	5.3	44
61	Characterization of the Dizinc Analogue of the Synthetic Diiron Protein DF1 Using ab Initio and Hybrid Quantum/Classical Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2003, 107, 4182-4188.	2.6	43
62	A Variational Definition of Electrostatic Potential Derived Charges. Journal of Physical Chemistry B, 2004, 108, 7963-7968.	2.6	40
63	Optimizing the Performance of Bias-Exchange Metadynamics: Folding a 48-Residue LysM Domain Using a Coarse-Grained Model. Journal of Physical Chemistry B, 2010, 114, 3259-3265.	2.6	40
64	Optimal Langevin modeling of out-of-equilibrium molecular dynamics simulations. Journal of Chemical Physics, 2008, 129, 074105.	3.0	39
65	A comparative theoretical study of dipeptide solvation in water. Journal of Computational Chemistry, 2006, 27, 672-684.	3.3	37
66	Free Energyab InitioMetadynamics:Â A New Tool for the Theoretical Study of Organometallic Reactivity? Example of the Câ^'C and Câ^'H Reductive Eliminations from Platinum(IV) Complexes. Organometallics, 2007, 26, 1241-1249.	2.3	37
67	Computing the Free Energy without Collective Variables. Journal of Chemical Theory and Computation, 2018, 14, 1206-1215.	5.3	37
68	The Energy Gap as a Universal Reaction Coordinate for the Simulation of Chemical Reactions. Journal of Physical Chemistry B, 2009, 113, 7867-7873.	2.6	36
69	A structural, functional, and computational analysis suggests pore flexibility as the base for the poor selectivity of CNG channels. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E3619-28.	7.1	35
70	Computing Free Energies and Accelerating Rare Events with Metadynamics. , 2006, , 315-347.		34
71	Shape and area fluctuation effects on nucleation theory. Journal of Chemical Physics, 2014, 140, 094501.	3.0	34
72	METAGUI 3: A graphical user interface for choosing the collective variables in molecular dynamics simulations. Computer Physics Communications, 2017, 217, 204-209.	7.5	34

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73	Predicting the Affinity of Peptides to Major Histocompatibility Complex Class II by Scoring Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2019, 59, 3464-3473.	5.4	34
74	A consensus protocol for the in silico optimisation of antibody fragments. Chemical Communications, 2019, 55, 14043-14046.	4.1	32
75	Binding affinity prediction of nanobodyâ€“protein complexes by scoring of molecular dynamics trajectories. Physical Chemistry Chemical Physics, 2018, 20, 3438-3444.	2.8	31
76	Force Generation in Lamellipodia Is a Probabilistic Process with Fast Growth and Retraction Events. Biophysical Journal, 2010, 98, 979-988.	0.5	29
77	Molecular dynamics simulation of reconstructive phase transitions on an anhydrous zeolite. Physical Review B, 2004, 70, .	3.2	28
78	Advillin Folding Takes Place on a Hypersurface of Small Dimensionality. Physical Review Letters, 2008, 101, 208101.	7.8	27
79	A fingerprint of surface-tension anisotropy in the free-energy cost of nucleation. Journal of Chemical Physics, 2013, 138, 064508.	3.0	27
80	A Candidate Ion-Retaining State in the Inward-Facing Conformation of Sodium/Galactose Symporter: Clues from Atomistic Simulations. Journal of Chemical Theory and Computation, 2013, 9, 1240-1246.	5.3	26
81	Which similarity measure is better for analyzing protein structures in a molecular dynamics trajectory?. Physical Chemistry Chemical Physics, 2011, 13, 10421.	2.8	25
82	Automatic topography of high-dimensional data sets by non-parametric density peak clustering. Information Sciences, 2021, 560, 476-492.	6.9	25
83	Conformations of the Huntingtin N-term in aqueous solution from atomistic simulations. FEBS Letters, 2011, 585, 3086-3089.	2.8	24
84	Designing Short Peptides with High Affinity for Organic Molecules: A Combined Docking, Molecular Dynamics, And Monte Carlo Approach. Journal of Chemical Theory and Computation, 2012, 8, 1121-1128.	5.3	24
85	Metadynamics surfing on topology barriers: the CP Nâ€˜1 case. Journal of High Energy Physics, 2016, 2016, 1.	4.7	24
86	Permeability Coefficients of Lipophilic Compounds Estimated by Computer Simulations. Journal of Chemical Theory and Computation, 2016, 12, 4093-4099.	5.3	22
87	Copper binding sites in the Câ€terminal domain of mouse prion protein: A hybrid (QM/MM) molecular dynamics study. Proteins: Structure, Function and Bioinformatics, 2008, 70, 1084-1098.	2.6	21
88	Spontaneously Forming Dendritic Voids in Liquid Water Can Host Small Polymers. Journal of Physical Chemistry Letters, 2019, 10, 5585-5591.	4.6	21
89	BACHSCORE. A tool for evaluating efficiently and reliably the quality of large sets of protein structures. Computer Physics Communications, 2013, 184, 2860-2865.	7.5	20
90	Metadynamics Simulations Reveal a Na+ Independent Exiting Path of Galactose for the Inward-Facing Conformation of vSGLT. PLoS Computational Biology, 2014, 10, e1004017.	3.2	20

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91	Computational design of cyclic peptides for the customized oriented immobilization of globular proteins. Physical Chemistry Chemical Physics, 2017, 19, 2740-2748.	2.8	20
92	Peptide biosensors for anticancer drugs: Design in silico to work in denaturizing environment. Biosensors and Bioelectronics, 2018, 100, 298-303.	10.1	20
93	The Subtle Trade-Off between Evolutionary and Energetic Constraints in Proteinâ€“Protein Interactions. Journal of Physical Chemistry Letters, 2019, 10, 1489-1497.	4.6	20
94	The intrinsic dimension of protein sequence evolution. PLoS Computational Biology, 2019, 15, e1006767.	3.2	19
95	Assessing the capability ofin silicomutation protocols for predicting the finite temperature conformation of amino acids. Physical Chemistry Chemical Physics, 2018, 20, 25901-25909.	2.8	18
96	Candidate Binding Sites for Allosteric Inhibition of the SARS-CoV-2 Main Protease from the Analysis of Large-Scale Molecular Dynamics Simulations. Journal of Physical Chemistry Letters, 2021, 12, 65-72.	4.6	18
97	Dynamical landscape and multistability of a climate model. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2021, 477, 20210019.	2.1	18
98	Native fold and docking pose discrimination by the same residueâ€based scoring function. Proteins: Structure, Function and Bioinformatics, 2015, 83, 621-630.	2.6	17
99	Designing High-Affinity Peptides for Organic Molecules by Explicit Solvent Molecular Dynamics. Journal of Physical Chemistry B, 2015, 119, 12963-12969.	2.6	17
100	Data segmentation based on the local intrinsic dimension. Scientific Reports, 2020, 10, 16449.	3.3	17
101	Ab Initio Simulations of Lewis-Acid-Catalyzed Hydrosilylation of Alkynes. ChemPhysChem, 2005, 6, 1772-1775.	2.1	15
102	Are structural biases at protein termini a signature of vectorial folding?. Proteins: Structure, Function and Bioinformatics, 2005, 62, 17-23.	2.6	15
103	Tracing the Entropy along a Reactive Pathway: The Energy As a Generalized Reaction Coordinate. Journal of Chemical Theory and Computation, 2009, 5, 2193-2196.	5.3	15
104	Sampling Molecular Conformers in Solution with Quantum Mechanical Accuracy at a Nearly Molecular-Mechanics Cost. Journal of Chemical Theory and Computation, 2016, 12, 4385-4389.	5.3	15
105	Explicit Characterization of the Free-Energy Landscape of a Protein in the Space of All Its C_{Î±} Carbons. Journal of Chemical Theory and Computation, 2020, 16, 80-87.	5.3	15
106	Brain network dynamics during spontaneous strategy shifts and incremental task optimization. NeuroImage, 2020, 217, 116854.	4.2	15
107	In Silico Design of Short Peptides as Sensing Elements for Phenolic Compounds. ACS Sensors, 2016, 1, 279-286.	7.8	14
108	Metadynamics: A Unified Framework for Accelerating Rare Events and Sampling Thermodynamics and Kinetics. , 2020, , 565-595.		13

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109	Ranking the information content of distance measures. , 2022, 1, .		13
110	Deciphering the folding kinetics of transmembrane helical proteins. Proceedings of the National Academy of Sciences of the United States of America, 2000, 97, 14229-14234.	7.1	12
111	PARCE: Protocol for Amino acid Refinement through Computational Evolution. Computer Physics Communications, 2021, 260, 107716.	7.5	12
112	A QUICKSTEP-based quantum mechanics/molecular mechanics approach for silica. Journal of Chemical Physics, 2006, 124, 154707.	3.0	11
113	Finite Temperature Properties of Clusters by Replica Exchange Metadynamics: The Water Nonamer. Journal of the American Chemical Society, 2011, 133, 2535-2540.	13.7	11
114	Protein-protein structure prediction by scoring molecular dynamics trajectories of putative poses. Proteins: Structure, Function and Bioinformatics, 2016, 84, 1312-1320.	2.6	11
115	Metadynamics: A Unified Framework for Accelerating Rare Events and Sampling Thermodynamics and Kinetics. , 2018, , 1-31.		11
116	Theory of the reentrant quantum rotational phase transition in high-pressure HD. Physical Review B, 2011, 84, .	3.2	10
117	Designing Short Peptides with High Affinity for Organic Molecules: A Combined Docking, Molecular Dynamics and Monte Carlo Approach. Biophysical Journal, 2013, 104, 556a.	0.5	10
118	Fusing simulation and experiment: The effect of mutations on the structure and activity of the influenza fusion peptide. Scientific Reports, 2016, 6, 28099.	3.3	10
119	Absolute Transition Rates for Rare Events from Dynamical Decoupling of Reaction Variables. Physical Review Letters, 2012, 109, 150601.	7.8	9
120	Non-Markovian effects on protein sequence evolution due to site dependent substitution rates. BMC Bioinformatics, 2016, 17, 258.	2.6	7
121	Vibrational entropy estimation can improve binding affinity prediction for nonâ€obligatory protein complexes. Proteins: Structure, Function and Bioinformatics, 2018, 86, 393-404.	2.6	7
122	Automatic classification of single-molecule force spectroscopy traces from heterogeneous samples. Bioinformatics, 2020, 36, 5014-5020.	4.1	7
123	Multiple-Allele MHC Class II Epitope Engineering by a Molecular Dynamics-Based Evolution Protocol. Frontiers in Immunology, 2022, 13, 862851.	4.8	7
124	A third hypothesis on the origin of the redshift: Application to the Pioneer 6 data. Physics Letters, Section A: General, Atomic and Solid State Physics, 1995, 209, 277-284.	2.1	6
125	QMMMW: A wrapper for QM/MM simulations with Quantum ESPRESSO Âand LAMMPS. Computer Physics Communications, 2015, 195, 191-198.	7.5	6
126	fMRI single trial discovery of spatioâ€temporal brain activity patterns. Human Brain Mapping, 2017, 38, 1421-1437.	3.6	6

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127	Protein Folding and Ligand-Enzyme Binding from Bias-Exchange Metadynamics Simulations. Current Physical Chemistry, 2012, 2, 79-91.	0.2	6
128	Quantum theory of frequency shifts of an electromagnetic wave interacting with a plasma. Physical Review E, 1997, 55, 7457-7461.	2.1	5
129	Markov state modeling of sliding friction. Physical Review E, 2016, 94, 053001.	2.1	5
130	New views on phototransduction from atomic force microscopy and single molecule force spectroscopy on native rods. Scientific Reports, 2017, 7, 12000.	3.3	5
131	Toward a unified scoring function for native state discrimination and drug-binding pocket recognition. Physical Chemistry Chemical Physics, 2018, 20, 17148-17155.	2.8	5
132	Model Folded Hydrophobic Polymers Reside in Highly Branched Voids. Journal of Physical Chemistry Letters, 2022, 13, 183-189.	4.6	5
133	Calculating thermodynamics properties of quantum systems by a non-Markovian Monte Carlo procedure. Physical Review E, 2009, 80, 015702.	2.1	4
134	Preface: Special Topic on Enhanced Sampling for Molecular Systems. Journal of Chemical Physics, 2018, 149, 072001.	3.0	4
135	A common root for coevolution and substitution rate variability in protein sequence evolution. Scientific Reports, 2019, 9, 18032.	3.3	4
136	A Rosetta-based protein design protocol converging to natural sequences. Journal of Chemical Physics, 2021, 154, 074114.	3.0	4
137	Statistically unbiased free energy estimates from biased simulations. Molecular Physics, 2021, 119, .	1.7	4
138	Computational Evolution Protocol for Peptide Design. Methods in Molecular Biology, 2022, 2405, 335-359.	0.9	3
139	ELECTRON TRANSFER INDUCED DISSOCIATION OF CHLORO-CYANO-BENZENE RADICAL ANION: DRIVING CHEMICAL REACTIONS VIA CHARGE RESTRAINTS. Journal of Theoretical and Computational Chemistry, 2005, 04, 985-999.	1.8	2
140	Simulation of Amyloid Nucleation with Bias-Exchange Metadynamics. Biophysical Journal, 2012, 102, 242a.	0.5	2
141	Interacting hard-core bosons and surface physics. Surface Science, 1997, 377-379, 514-518.	1.9	1
142	Interacting hard-core bosons and surface preroughening. Physical Review B, 1998, 58, 13151-13162.	3.2	1
143	Thermodynamics of an Intrinsically Disordered Protein by Atomistic Simulations. Biophysical Journal, 2013, 104, 55a.	0.5	1
144	A Markov state modeling analysis of sliding dynamics of a 2D model. Journal of Chemical Physics, 2017, 147, 152721.	3.0	1

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145	Predicting Amino Acid Substitution Probabilities Using Single Nucleotide Polymorphisms. Genetics, 2017, 207, 643-652.	2.9	1
146	The permeation mechanism of organic cations through a CNG mimic channel. PLoS Computational Biology, 2018, 14, e1006295.	3.2	1
147	Density Peak clustering of protein sequences associated to a Pfam clan reveals clear similarities and interesting differences with respect to manual family annotation. BMC Bioinformatics, 2021, 22, 121.	2.6	1
148	Stepâ€“step interactions and correlations from 1D hard-core boson mapping. Surface Science, 1998, 402-404, 880-885.	1.9	0
149	QM/MM Simulation of the First Step of Vision. , 2005, , 237-243.		0
150	Sodium-Galactose Transporter: The First Steps of the Transport Mechanism Investigated by Molecular Dynamics. Biophysical Journal, 2014, 106, 365a-366a.	0.5	0
151	Mechanism of Ionic Permeation in the Mimics of CNG Channels: A Structural, Functional and Computational Analysis. Biophysical Journal, 2014, 106, 758a.	0.5	0
152	Computational Design of Peptides Bound to the Major Histocompatibility Complex Class II. Biophysical Journal, 2020, 118, 359a.	0.5	0
153	Improving acute stroke assessment in non-enhanced CT: Automated tool for early ischemic lesion volume detection. Journal of the Neurological Sciences, 2021, 429, 119611.	0.6	0
154	When kinetics plays strange tricks. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, e2122078119.	7.1	0