Giovanni Bussi

List of Publications by Year
in descending order

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Version: 2024-02-01

103 papers	24,902 citations	87401 40 h-index	37326 100 g-index
120 all docs	120 docs citations	120 times ranked	25524 citing authors

#	Article	IF	Citations
1	Molecular Dynamics of Solids at Constant Pressure and Stress Using Anisotropic Stochastic Cell Rescaling. Applied Sciences (Switzerland), 2022, 12, 1139.	1.3	1
2	Toward Convergence in Folding Simulations of RNA Tetraloops: Comparison of Enhanced Sampling Techniques and Effects of Force Field Modifications. Journal of Chemical Theory and Computation, 2022, 18, 2642-2656.	2.3	34
3	Automatic Learning of Hydrogen-Bond Fixes in the AMBER RNA Force Field. Journal of Chemical Theory and Computation, 2022, 18, 4490-4502.	2.3	21
4	Conformational Ensembles of Noncoding Elements in the SARS-CoV-2 Genome from Molecular Dynamics Simulations. Journal of the American Chemical Society, 2021, 143, 8333-8343.	6.6	17
5	Arginine multivalency stabilizes protein/RNA condensates. Protein Science, 2021, 30, 1418-1426.	3.1	18
6	Reweighting of molecular simulations with explicit-solvent SAXS restraints elucidates ion-dependent RNA ensembles. Nucleic Acids Research, 2021, 49, e84-e84.	6.5	25
7	Comparing state-of-the-art approaches to back-calculate SAXS spectra from atomistic molecular dynamics simulations. European Physical Journal B, 2021, 94, 1.	0.6	12
8	Conformational ensembles of an RNA hairpin using molecular dynamics and sparse NMR data. Nucleic Acids Research, 2020, 48, 1164-1174.	6.5	28
9	Pressure control using stochastic cell rescaling. Journal of Chemical Physics, 2020, 153, 114107.	1.2	113
10	Directional translocation resistance of Zika xrRNA. Nature Communications, 2020, 11, 3749.	5.8	15
11	Fine-Tuning of the AMBER RNA Force Field with a New Term Adjusting Interactions of Terminal Nucleotides. Journal of Chemical Theory and Computation, 2020, 16, 3936-3946.	2.3	39
12	Toward empirical force fields that match experimental observables. Journal of Chemical Physics, 2020, 152, 230902.	1.2	49
13	Assessing the accuracy of direct-coupling analysis for RNA contact prediction. Rna, 2020, 26, 637-647.	1.6	20
14	Using metadynamics to explore complex free-energy landscapes. Nature Reviews Physics, 2020, 2, 200-212.	11.9	346
15	Metadynamics: A Unified Framework for Accelerating Rare Events and Sampling Thermodynamics and Kinetics. , 2020, , 565-595.		13
16	Machine learning a model for RNA structure prediction. NAR Genomics and Bioinformatics, 2020, 2, lqaa090.	1.5	19
17	Asymmetric base-pair opening drives helicase unwinding dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 22471-22477.	3.3	15
18	Fitting Corrections to an RNA Force Field Using Experimental Data. Journal of Chemical Theory and Computation, 2019, 15, 3425-3431.	2.3	54

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19	The mechanism of RNA base fraying: Molecular dynamics simulations analyzed with core-set Markov state models. Journal of Chemical Physics, 2019, 150, 154123.	1.2	24
20	Statistical mechanical properties of sequence space determine the efficiency of the various algorithms to predict interaction energies and native contacts from protein coevolution.. Physical Biology, 2019, 16, 046007.	0.8	4
21	Improving the Performance of the Amber RNA Force Field by Tuning the Hydrogen-Bonding Interactions. Journal of Chemical Theory and Computation, 2019, 15, 3288-3305.	2.3	97
22	Barnaba: software for analysis of nucleic acid structures and trajectories. Rna, 2019, 25, 219-231.	1.6	50
23	Analyzing and Biasing Simulations with PLUMED. Methods in Molecular Biology, 2019, 2022, 529-578.	0.4	49
24	Structural determinants of the SINE B2 element embedded in the long non-coding RNA activator of translation AS Uchl1. Scientific Reports, 2018, 8, 3189.	1.6	32
25	Exploring RNA structure and dynamics through enhanced sampling simulations. Current Opinion in Structural Biology, 2018, 49, 63-71.	2.6	47
26	Automated Force-Field Parametrization Guided by Multisystem Ensemble Averages. Biophysical Journal, 2018, 114, 437a.	0.2	0
27	Effects and limitations of a nucleobase-driven backmapping procedure for nucleic acids using steered molecular dynamics. Biochemical and Biophysical Research Communications, 2018, 498, 352-358.	1.0	8
28	Molecular Dynamics Simulations Reveal an Interplay between SHAPE Reagent Binding and RNA Flexibility. Journal of Physical Chemistry Letters, 2018, 9, 313-318.	2.1	30
29	A nucleobase-centered coarse-grained representation for structure prediction of RNA motifs. Nucleic Acids Research, 2018, 46, 1674-1683.	6.5	31
30	RNA Structural Dynamics As Captured by Molecular Simulations: A Comprehensive Overview. Chemical Reviews, 2018, 118, 4177-4338.	23.0	408
31	Determination of Structural Ensembles of Proteins: Restraining vs Reweighting. Journal of Chemical Theory and Computation, 2018, 14, 6632-6641.	2.3	54
32	Metadynamics: A Unified Framework for Accelerating Rare Events and Sampling Thermodynamics and Kinetics. , 2018, , 1-31.		11
33	Atomistic Details of Chymotrypsin Conformational Changes upon Adsorption on Silica. ACS Biomaterials Science and Engineering, 2018, 4, 4036-4050.	2.6	15
34	Conformational ensembles of RNA oligonucleotides from integrating NMR and molecular simulations. Science Advances, 2018, 4, eaar8521.	4.7	99
35	Using the Maximum Entropy Principle to Combine Simulations and Solution Experiments. Computation, 2018, 6, 15.	1.0	107
36	Understanding in-line probing experiments by modeling cleavage of nonreactive RNA nucleotides. Rna, 2017, 23, 712-720.	1.6	10

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37	Unraveling Mg²⁺â€“RNA binding with atomistic molecular dynamics. Rna, 2017, 23, 628-638.	1.6	61
38	Exploring the Dynamics of Propeller Loops in Human Telomeric DNA Quadruplexes Using Atomistic Simulations. Journal of Chemical Theory and Computation, 2017, 13, 2458-2480.	2.3	39
39	Predicting the Kinetics of RNA Oligonucleotides Using Markov State Models. Journal of Chemical Theory and Computation, 2017, 13, 926-934.	2.3	26
40	Fibrillation-prone conformations of the amyloid-Î²-42 peptide at the gold/water interface. Nanoscale, 2017, 9, 2279-2290.	2.8	25
41	Folding of guanine quadruplex moleculesâ€“funnel-like mechanism or kinetic partitioning? An overview from MD simulation studies. Biochimica Et Biophysica Acta - General Subjects, 2017, 1861, 1246-1263.	1.1	89
42	Combining Simulations and Solution Experiments as a Paradigm for RNA Force Field Refinement. Journal of Chemical Theory and Computation, 2016, 12, 6192-6200.	2.3	94
43	Empirical Corrections to the Amber RNA Force Field with Target Metadynamics. Journal of Chemical Theory and Computation, 2016, 12, 2790-2798.	2.3	54
44	RNA Conformational Fluctuations from Elastic Network Models: A Comparison with Molecular Dynamics and Shape Experiments. Biophysical Journal, 2016, 110, 330a.	0.2	0
45	RNA Conformational Ensembles: Narrowing the GAP between Experiments and Simulations with Metadynamics. Biophysical Journal, 2016, 110, 522a-523a.	0.2	0
46	Free Energy Landscape of GAGA and UUCG RNA Tetraloops. Journal of Physical Chemistry Letters, 2016, 7, 4032-4038.	2.1	70
47	Computer Folding of RNA Tetraloops: Identification of Key Force Field Deficiencies. Journal of Chemical Theory and Computation, 2016, 12, 4534-4548.	2.3	125
48	RNA folding pathways in stop motion. Nucleic Acids Research, 2016, 44, 5883-5891.	6.5	38
49	A Nucleobase-Centric Coarse-Grained Model for Structure Prediction of RNA Fragments. Biophysical Journal, 2015, 108, 235a.	0.2	0
50	Kissing loop interaction in adenine riboswitch: insights from umbrella sampling simulations. BMC Bioinformatics, 2015, 16, S6.	1.2	28
51	ATP dependent NS3 helicase interaction with RNA: insights from molecular simulations. Nucleic Acids Research, 2015, 43, 8725-8734.	6.5	27
52	Elastic network models for RNA: a comparative assessment with molecular dynamics and SHAPE experiments. Nucleic Acids Research, 2015, 43, 7260-7269.	6.5	47
53	Enhanced Conformational Sampling Using Replica Exchange with Collective-Variable Tempering. Journal of Chemical Theory and Computation, 2015, 11, 1077-1085.	2.3	87
54	Using Reweighted Pulling Simulations to Characterize Conformational Changes in Riboswitches. Methods in Enzymology, 2015, 553, 139-162.	0.4	15

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55	Hairpins participating in folding of human telomeric sequence quadruplexes studied by standard and T-REMD simulations. Nucleic Acids Research, 2015, 43, gkv994.	6.5	47
56	Accurate Multiple Time Step in Biased Molecular Simulations. Journal of Chemical Theory and Computation, 2015, 11, 139-146.	2.3	31
57	Enhanced Sampling in Molecular Dynamics Using Metadynamics, Replica-Exchange, and Temperature-Acceleration. Entropy, 2014, 16, 163-199.	1.1	367
58	The role of nucleobase interactions in RNA structure and dynamics. Nucleic Acids Research, 2014, 42, 13306-13314.	6.5	127
59	Hamiltonian replica exchange in GROMACS: a flexible implementation. Molecular Physics, 2014, 112, 379-384.	0.8	186
60	Role of Magnesium Ions and Ligand Stacking in the Adenine Riboswitch Folding. Biophysical Journal, 2014, 106, 285a.	0.2	1
61	PLUMED 2: New feathers for an old bird. Computer Physics Communications, 2014, 185, 604-613.	3.0	2,454
62	Bowl Inversion of Surface-Adsorbed Sumanene. Journal of the American Chemical Society, 2014, 136, 13666-13671.	6.6	36
63	Probing Riboswitch Binding Sites with Molecular Docking, Focused Libraries, and In-line Probing Assays. Methods in Molecular Biology, 2014, 1103, 141-151.	0.4	5
64	Ligand-induced stabilization of the aptamer terminal helix in the add adenine riboswitch. Rna, 2013, 19, 1517-1524.	1.6	43
65	Structural Role of Uracil DNA Glycosylase for the Recognition of Uracil in DNA Duplexes. Clues from Atomistic Simulations. Journal of Chemical Information and Modeling, 2013, 53, 1371-1387.	2.5	4
66	RNA/Peptide Binding Driven by Electrostaticsâ€”Insight from Bidirectional Pulling Simulations. Journal of Chemical Theory and Computation, 2013, 9, 1720-1730.	2.3	48
67	RNA Unwinding from Reweighted Pulling Simulations. Journal of the American Chemical Society, 2012, 134, 5173-5179.	6.6	40
68	Role of the Subunit Interactions in the Conformational Transitions in Adult Human Hemoglobin: An Explicit Solvent Molecular Dynamics Study. Journal of Physical Chemistry B, 2012, 116, 11004-11009.	1.2	21
69	Metadynamics with Adaptive Gaussians. Journal of Chemical Theory and Computation, 2012, 8, 2247-2254.	2.3	220
70	Understanding CNG Channels Gating Process by MD Simulations. Biophysical Journal, 2012, 102, 129a-130a.	0.2	0
71	Ab initiocomplex band structure of conjugated polymers: Effects of hydrid density functional theory and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="italic">GW</mml:mi></mml:mrow></mml:math>schemes. Physical Review B, 2012, 85, .	1.1	34
72	Nonkinetic Modeling of the Mechanical Unfolding of Multimodular Proteins: Theory and Experiments. Biophysical Journal, 2011, 101, 1504-1512.	0.2	7

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73	Reactive force field simulation of proton diffusion in BaZrO₃using an empirical valence bond approach. Journal of Physics Condensed Matter, 2011, 23, 334213.	0.7	31
74	Unraveling effects of disorder on the electronic structure of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msu first principles. Physical Review B, 2010, 81, .	1.1	22
75	Colored-Noise Thermostats Ã la Carte. Journal of Chemical Theory and Computation, 2010, 6, 1170-1180.	2.3	199
76	Isothermal-isobaric molecular dynamics using stochastic velocity rescaling. Journal of Chemical Physics, 2009, 130, 074101.	1.2	297
77	PLUMED: A portable plugin for free-energy calculations with molecular dynamics. Computer Physics Communications, 2009, 180, 1961-1972.	3.0	1,448
78	SaX: An open source package for electronic-structure and optical-properties calculations in the GW approximation. Computer Physics Communications, 2009, 180, 1416-1425.	3.0	38
79	Transâ^'cis Switching Mechanisms in Proline Analogues and Their Relevance for the Gating of the 5-HT₃ Receptor. Journal of Physical Chemistry B, 2009, 113, 12148-12153.	1.2	44
80	Langevin Equation with Colored Noise for Constant-Temperature Molecular Dynamics Simulations. Physical Review Letters, 2009, 102, 020601.	2.9	170
81	Nuclear Quantum Effects in Solids Using a Colored-Noise Thermostat. Physical Review Letters, 2009, 103, 030603.	2.9	188
82	Ensemble of Transition State Structures for the Cisâ^'Trans Isomerization of N-Methylacetamide. Journal of Physical Chemistry B, 2009, 113, 12521-12529.	1.2	23
83	Unravelling the Shuttling Mechanism in a Photoswitchable Multicomponent Bistable Rotaxane. Angewandte Chemie - International Edition, 2008, 47, 3536-3539.	7.2	64
84	Stochastic thermostats: comparison of local and global schemes. Computer Physics Communications, 2008, 179, 26-29.	3.0	112
85	Well-Tempered Metadynamics: A Smoothly Converging and Tunable Free-Energy Method. Physical Review Letters, 2008, 100, 020603.	2.9	2,201
86	Optimal Langevin modeling of out-of-equilibrium molecular dynamics simulations. Journal of Chemical Physics, 2008, 129, 074105.	1.2	39
87	Conjugate gradient heat bath for ill-conditioned actions. Physical Review E, 2007, 76, 026707.	0.8	2
88	Accurate sampling using Langevin dynamics. Physical Review E, 2007, 75, 056707.	0.8	257
89	Canonical sampling through velocity rescaling. Journal of Chemical Physics, 2007, 126, 014101.	1.2	11,867
90	Free-Energy Landscape for Î² Hairpin Folding from Combined Parallel Tempering and Metadynamics. Journal of the American Chemical Society, 2006, 128, 13435-13441.	6.6	458

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91	Equilibrium Free Energies from Nonequilibrium Metadynamics. Physical Review Letters, 2006, 96, 090601.	2.9	355
92	Ab-initio study of excitonic effects in conventional and organic semiconductors. Physica Status Solidi (B): Basic Research, 2005, 242, 1754-1758.	0.7	14
93	Light-Emitting Polymers: a First-Principles Analysis of Singlet-Exciton Harvesting in PPV. AIP Conference Proceedings, 2005, , .	0.3	0
94	A symmetrized-basis approach to excitons in carbon nanotubes. AIP Conference Proceedings, 2005, , .	0.3	0
95	Quantum interferences in the Raman cross section for the radial breathing mode in metallic carbon nanotubes. Physical Review B, 2005, 71, .	1.1	21
96	First-principles approach for the calculation of optical properties of one-dimensional systems with helical symmetry: The case of carbon nanotubes. Physical Review B, 2005, 72, .	1.1	33
97	Ab initiostudy of transport parameters in polymer crystals. Physical Review B, 2004, 69, .	1.1	25
98	Excitons in Carbon Nanotubes: AnAb InitioSymmetry-Based Approach. Physical Review Letters, 2004, 92, 196401.	2.9	269
99	Effects of the Electron?Hole Interaction on the Optical Properties of Materials: the Bethe?Salpeter Equation. Physica Scripta, 2004, T109, 141.	1.2	18
100	Relationship between structural and optoelectronic properties in semiconducting polymers. Semiconductor Science and Technology, 2004, 19, S362-S364.	1.0	4
101	Charge transport and radiative recombination in polythiophene crystals: a first-principles study. Synthetic Metals, 2003, 139, 755-757.	2.1	6
102	Solid State Effects on Exciton States and Optical Properties of PPV. Physical Review Letters, 2002, 88, 206403.	2.9	152
103	Interchain interaction and Davydov splitting in polythiophene crystals: An ab initio approach. Applied Physics Letters, 2002, 80, 4118-4120.	1.5	51