Stefano Piana

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/10761999/publications.pdf

Version: 2024-02-01

41 papers	15,339 citations	145106 33 h-index	340414 39 g-index
42 all docs	42 docs citations	42 times ranked	16419 citing authors

#	Article	IF	Citations
1	Development of Force Field Parameters for the Simulation of Single- and Double-Stranded DNA Molecules and DNAâ€“Protein Complexes. Journal of Physical Chemistry B, 2022, 126, 4442-4457.	1.2	25
2	Development of a Force Field for the Simulation of Single-Chain Proteins and Proteinâ€“Protein Complexes. Journal of Chemical Theory and Computation, 2020, 16, 2494-2507.	2.3	104
3	Mechanism of Coupled Folding-upon-Binding of an Intrinsically Disordered Protein. Journal of the American Chemical Society, 2020, 142, 11092-11101.	6.6	81
4	RNA force field with accuracy comparable to state-of-the-art protein force fields. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E1346-E1355.	3.3	214
5	Atomic-Level Description of Protein Folding inside the GroEL Cavity. Journal of Physical Chemistry B, 2018, 122, 11440-11449.	1.2	10
6	Developing a molecular dynamics force field for both folded and disordered protein states. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E4758-E4766.	3.3	738
7	Assessment of the utility of contactâ€based restraints in accelerating the prediction of protein structure using molecular dynamics simulations. Protein Science, 2016, 25, 19-29.	3.1	26
8	Picosecond to Millisecond Structural Dynamics in Human Ubiquitin. Journal of Physical Chemistry B, 2016, 120, 8313-8320.	1.2	93
9	Demonstrating an Order-of-Magnitude Sampling Enhancement in Molecular Dynamics Simulations of Complex Protein Systems. Journal of Chemical Theory and Computation, 2016, 12, 1360-1367.	2.3	79
10	Identifying localized changes in large systems: Change-point detection for biomolecular simulations. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 7454-7459.	3.3	24
11	Interaction Networks in Protein Folding via Atomic-Resolution Experiments and Long-Time-Scale Molecular Dynamics Simulations. Journal of the American Chemical Society, 2015, 137, 6506-6516.	6.6	76
12	Water Dispersion Interactions Strongly Influence Simulated Structural Properties of Disordered Protein States. Journal of Physical Chemistry B, 2015, 119, 5113-5123.	1.2	671
13	Assessing the accuracy of physical models used in protein-folding simulations: quantitative evidence from long molecular dynamics simulations. Current Opinion in Structural Biology, 2014, 24, 98-105.	2.6	424
14	Atomistic Description of the Folding of a Dimeric Protein. Journal of Physical Chemistry B, 2013, 117, 12935-12942.	1.2	45
15	Atomic-level description of ubiquitin folding. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 5915-5920.	3.3	281
16	Protein folding kinetics and thermodynamics from atomistic simulation. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 17845-17850.	3.3	262
17	Systematic Validation of Protein Force Fields against Experimental Data. PLoS ONE, 2012, 7, e32131.	1.1	570
18	Structure and Dynamics of an Unfolded Protein Examined by Molecular Dynamics Simulation. Journal of the American Chemical Society, 2012, 134, 3787-3791.	6.6	222

#	Article	IF	Citations
19	Refinement of protein structure homology models via long, allâ€atom molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2012, 80, 2071-2079.	1.5	226
20	Evaluating the Effects of Cutoffs and Treatment of Long-range Electrostatics in Protein Folding Simulations. PLoS ONE, 2012, 7, e39918.	1.1	83
21	How Robust Are Protein Folding Simulations with Respect to Force Field Parameterization?. Biophysical Journal, 2011, 100, L47-L49.	0.2	725
22	How Fast-Folding Proteins Fold. Science, 2011, 334, 517-520.	6.0	1,609
23	Computational Design and Experimental Testing of the Fastest-Folding Î²-Sheet Protein. Journal of Molecular Biology, 2011, 405, 43-48.	2.0	106
24	Atomic-Level Characterization of the Structural Dynamics of Proteins. Science, 2010, 330, 341-346.	6.0	1,583
25	Improved sideâ€chain torsion potentials for the Amber ff99SB protein force field. Proteins: Structure, Function and Bioinformatics, 2010, 78, 1950-1958.	1.5	4,694
26	Identification of two distinct inactive conformations of the Î² ₂ -adrenergic receptor reconciles structural and biochemical observations. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 4689-4694.	3.3	298
27	A Kinetic Model of Trp-Cage Folding from Multiple Biased Molecular Dynamics Simulations. PLoS Computational Biology, 2009, 5, e1000452.	1.5	246
28	Millisecond-scale molecular dynamics simulations on Anton. , 2009, , .		238
29	Drug resistance in HIV-1 protease: Flexibility-assisted mechanism of compensatory mutations. Protein Science, 2009, 11, 2393-2402.	3.1	124
30	Exploring the Folding Free Energy Landscape of Insulin Using Bias Exchange Metadynamics. Journal of Physical Chemistry B, 2009, 113, 3556-3564.	1.2	48
31	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.	2.0	49
32	Advillin Folding Takes Place on a Hypersurface of Small Dimensionality. Physical Review Letters, 2008, 101, 208101.	2.9	27
33	Atomistic Simulation of the DNA Helixâ^'Coil Transition. Journal of Physical Chemistry A, 2007, 111, 12349-12354.	1.1	28
34	A Bias-Exchange Approach to Protein Folding. Journal of Physical Chemistry B, 2007, 111, 4553-4559.	1.2	498
35	Simulating micrometre-scale crystal growth from solution. Nature, 2005, 438, 70-73.	13.7	201
36	Structure and energy of a DNA dodecamer under tensile load. Nucleic Acids Research, 2005, 33, 7029-7038.	6.5	43

#	Article	IF	Citations
37	Understanding the Barriers to Crystal Growth:Â Dynamical Simulation of the Dissolution and Growth of Urea from Aqueous Solution. Journal of the American Chemical Society, 2005, 127, 1975-1982.	6.6	113
38	Reaction Mechanism of HIV-1 Protease by Hybrid Car-Parrinello/Classical MD Simulations. Journal of Physical Chemistry B, 2004, 108, 11139-11149.	1.2	106
39	Role of Conformational Fluctuations in the Enzymatic Reaction of HIV-1 Protease. Journal of Molecular Biology, 2002, 319, 567-583.	2.0	130
40	Ab Initio Molecular Dynamics-Based Assignment of the Protonation State of Pepstatin A/HIV-1 Protease Cleavage Site. Journal of the American Chemical Society, 2001, 123, 8730-8737.	6.6	124
41	Conformational flexibility of the catalytic Asp dyad in HIV-1 protease: An ab initio study on the free enzyme. , 2000, 39, 26-36.		94