Stefano Piana

List of Publications by Citations

40 papers	11,891 citations	34 h-index	42 g-index
42 ext. papers	13,841 ext. citations	9.8 avg, IF	6.57 L-index

#	Paper	IF	Citations
40	Improved side-chain torsion potentials for the Amber ff99SB protein force field. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 1950-8	4.2	3395
39	Atomic-level characterization of the structural dynamics of proteins. *Science*, **2010**, 330, 341-6	33.3	1331
38	How fast-folding proteins fold. *Science*, **2011**, 334, 517-20	33.3	1284
37	How robust are protein folding simulations with respect to force field parameterization?. *Biophysical Journal*, **2011**, 100, L47-9	2.9	611
36	Systematic validation of protein force fields against experimental data. *PLoS ONE*, **2012**, 7, e32131	3.7	493
35	Water dispersion interactions strongly influence simulated structural properties of disordered protein states. *Journal of Physical Chemistry B*, **2015**, 119, 5113-23	3.4	468
34	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	11.5	434
33	A bias-exchange approach to protein folding. *Journal of Physical Chemistry B*, **2007**, 111, 4553-9	3.4	430
32	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	8.1	351
31	Identification of two distinct inactive conformations of the beta2-adrenergic receptor reconciles structural and biochemical observations. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 4689-94	11.5	247
30	Atomic-level description of ubiquitin folding. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 5915-20	11.5	242
29	Protein folding kinetics and thermodynamics from atomistic simulation. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 17845-50	11.5	221
28	A kinetic model of trp-cage folding from multiple biased molecular dynamics simulations. *PLoS Computational Biology*, **2009**, 5, e1000452	5	217
27	Structure and dynamics of an unfolded protein examined by molecular dynamics simulation. *Journal of the American Chemical Society*, **2012**, 134, 3787-91	16.4	193
26	Refinement of protein structure homology models via long, all-atom molecular dynamics simulations. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 2071-9	4.2	193
25	Simulating micrometre-scale crystal growth from solution. *Nature*, **2005**, 438, 70-3	50.4	177
24	Millisecond-scale molecular dynamics simulations on Anton **2009**,		166

23	Role of conformational fluctuations in the enzymatic reaction of HIV-1 protease. *Journal of Molecular Biology*, **2002**, 319, 567-83	6.5	122
22	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, 8730-7	16.4	117
21	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	11.5	114
20	Drug resistance in HIV-1 protease: Flexibility-assisted mechanism of compensatory mutations. *Protein Science*, **2002**, 11, 2393-402	6.3	105
19	Reaction Mechanism of HIV-1 Protease by Hybrid Car-Parrinello/Classical MD Simulations. *Journal of Physical Chemistry B*, **2004**, 108, 11139-11149	3.4	100
18	Computational design and experimental testing of the fastest-folding β-sheet protein. *Journal of Molecular Biology*, **2011**, 405, 43-8	6.5	94
17	Understanding the barriers to crystal growth: dynamical simulation of the dissolution and growth of urea from aqueous solution. *Journal of the American Chemical Society*, **2005**, 127, 1975-82	16.4	93
16	Conformational flexibility of the catalytic Asp dyad in HIV-1 protease: An ab initio study on the free enzyme. *Proteins: Structure, Function and Bioinformatics*, **2000**, 39, 26-36	4.2	90
15	Evaluating the effects of cutoffs and treatment of long-range electrostatics in protein folding simulations. *PLoS ONE*, **2012**, 7, e39918	3.7	72
14	Picosecond to Millisecond Structural Dynamics in Human Ubiquitin. *Journal of Physical Chemistry B*, **2016**, 120, 8313-20	3.4	70
13	Interaction Networks in Protein Folding via Atomic-Resolution Experiments and Long-Time-Scale Molecular Dynamics Simulations. *Journal of the American Chemical Society*, **2015**, 137, 6506-16	16.4	66
12	Demonstrating an Order-of-Magnitude Sampling Enhancement in Molecular Dynamics Simulations of Complex Protein Systems. *Journal of Chemical Theory and Computation*, **2016**, 12, 1360-7	6.4	58
11	Development of a Force Field for the Simulation of Single-Chain Proteins and Protein-Protein Complexes. *Journal of Chemical Theory and Computation*, **2020**, 16, 2494-2507	6.4	46
10	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, 460-70	6.5	45
9	Exploring the folding free energy landscape of insulin using bias exchange metadynamics. *Journal of Physical Chemistry B*, **2009**, 113, 3556-64	3.4	42
8	Structure and energy of a DNA dodecamer under tensile load. *Nucleic Acids Research*, **2005**, 33, 7029-38	20.1	40
7	Atomistic description of the folding of a dimeric protein. *Journal of Physical Chemistry B*, **2013**, 117, 12935-42	3.4	37
6	Mechanism of Coupled Folding-upon-Binding of an Intrinsically Disordered Protein. *Journal of the American Chemical Society*, **2020**, 142, 11092-11101	16.4	26

5	Assessment of the utility of contact-based restraints in accelerating the prediction of protein structure using molecular dynamics simulations. *Protein Science*, **2016**, 25, 19-29	6.3	24
4	Advillin folding takes place on a hypersurface of small dimensionality. *Physical Review Letters*, **2008**, 101, 208101	7.4	23
3	Atomistic simulation of the DNA helix-coil transition. *Journal of Physical Chemistry A*, **2007**, 111, 12349-54	2.8	20
2	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, 7454-9	11.5	17
1	Atomic-Level Description of Protein Folding inside the GroEL Cavity. *Journal of Physical Chemistry B*, **2018**, 122, 11440-11449	3.4	9