Francesco Rao

List of Publications by Year in Descending Order

30 papers	1,467 citations	16 h-index	30 g-index
30 ext. papers	1,575 ext. citations	5 avg, IF	4.53 L-index

#	Paper	IF	Citations
30	A comparative analysis of clustering algorithms: O2 migration in truncated hemoglobin I from transition networks. *Journal of Chemical Physics*, **2015**, 142, 025103	3.9	9
29	A hydro-kinetic scheme for the dynamics of hydrogen bonds in water-like fluids. *Physical Chemistry Chemical Physics*, **2014**, 16, 15510-8	3.6	3
28	Topological dynamics in supramolecular rotors. *Nano Letters*, **2014**, 14, 4461-8	11.5	28
27	Network analysis of proton transfer in liquid water. *Journal of Chemical Physics*, **2014**, 140, 244502	3.9	11
26	Structure and dynamics of water in crowded environments slows down peptide conformational changes. *Journal of Chemical Physics*, **2014**, 141, 045101	3.9	15
25	Structure-dynamics relationship in coherent transport through disordered systems. *Nature Communications*, **2013**, 4, 2296	17.4	20
24	The quest for self-consistency in hydrogen bond definitions. *Journal of Chemical Physics*, **2013**, 139, 084501	3.9	57
23	Lattice Boltzmann implementation of the three-dimensional Ben-Naim potential for water-like fluids. *Journal of Chemical Physics*, **2013**, 138, 124105	3.9	2
22	Consensus for the Fip35 folding mechanism?. *Journal of Chemical Physics*, **2013**, 139, 035102	3.9	16
21	Thermodynamics and kinetics of large-time-step molecular dynamics. *Journal of Computational Chemistry*, **2012**, 33, 475-83	3.5	10
20	Water structure-forming capabilities are temperature shifted for different models. *Journal of Physical Chemistry B*, **2012**, 116, 7538-43	3.4	12
19	Beyond the binding site: the role of the β3-β4 loop and extra-domain structures in PDZ domains. *PLoS Computational Biology*, **2012**, 8, e1002429	5	35
18	Towards a microscopic description of the free-energy landscape of water. *Journal of Chemical Physics*, **2012**, 137, 144504	3.9	18
17	Accounting for the kinetics in order parameter analysis: lessons from theoretical models and a disordered peptide. *Journal of Chemical Physics*, **2012**, 137, 194101	3.9	14
16	Three-dimensional infrared spectroscopy of isotope-substituted liquid water reveals heterogeneous dynamics. *Journal of Physical Chemistry B*, **2011**, 115, 6976-84	3.4	63
15	Wordom: a user-friendly program for the analysis of molecular structures, trajectories, and free energy surfaces. *Journal of Computational Chemistry*, **2011**, 32, 1183-94	3.5	187
14	Protein inherent structures by different minimization strategies. *Journal of Computational Chemistry*, **2011**, 32, 1113-6	3.5	4

13	Protein dynamics investigated by inherent structure analysis. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 9152-7	11.5	49
12	Structural inhomogeneity of water by complex network analysis. *Journal of Physical Chemistry B*, **2010**, 114, 15598-604	3.4	34
11	Local Transition Gradients Indicating the Global Attributes of Protein Energy Landscapes. *Journal of Physical Chemistry Letters*, **2010**, 1, 1580-1583	6.4	10
10	Computational Screening of Rhodopsin Mutations Associated with Retinitis Pigmentosa. *Journal of Chemical Theory and Computation*, **2009**, 5, 2472-85	6.4	12
9	Uncovering the topology of configuration space networks. *Physical Review E*, **2007**, 76, 026113	2.4	29
8	Wordom: a program for efficient analysis of molecular dynamics simulations. *Bioinformatics*, **2007**, 23, 2625-7	7.2	227
7	Estimation of folding probabilities and phi values from molecular dynamics simulations of reversible Peptide folding. *Methods in Molecular Biology*, **2007**, 350, 225-49	1.4	6
6	Estimation of protein folding probability from equilibrium simulations. *Journal of Chemical Physics*, **2005**, 122, 184901	3.9	32
5	Local modularity measure for network clusterizations. *Physical Review E*, **2005**, 72, 056107	2.4	87
4	Phi-value analysis by molecular dynamics simulations of reversible folding. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 628-33	11.5	63
3	Frequency-domain study of relaxation in the random orthogonal model. *Philosophical Magazine*, **2004**, 84, 1389-1395	1.6	
2	The protein folding network. *Journal of Molecular Biology*, **2004**, 342, 299-306	6.5	322
1	Replica exchange molecular dynamics simulations of reversible folding. *Journal of Chemical Physics*, **2003**, 119, 4035-4042	3.9	92