

# Vania Calandrini

## List of Publications by Year in descending order

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29  
papers

499  
citations

567281

15  
h-index

677142

22  
g-index

30  
all docs

30  
docs citations

30  
times ranked

701  
citing authors

#	ARTICLE	IF	CITATIONS
1	Subdiffusive-Brownian crossover in membrane proteins: a Generalized Langevin Equation-based approach. <i>Biophysical Journal</i> , 2021, 120, 4722-4737.	0.5	6
2	Hydrodynamics of immiscible binary fluids with viscosity contrast: a multiparticle collision dynamics approach. <i>Soft Matter</i> , 2021, 17, 7978-7990.	2.7	3
3	Open-Boundary Molecular Mechanics/Coarse-Grained Framework for Simulations of Low-Resolution G-Protein-Coupled Receptor-Ligand Complexes. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2101-2109.	5.3	16
4	Molecular Dynamics Simulations of the [2Fe-2S] Cluster-Binding Domain of NEET Proteins Reveal Key Molecular Determinants That Induce Their Cluster Transfer/Release. <i>Journal of Physical Chemistry B</i> , 2017, 121, 10648-10656.	2.6	18
5	Open Boundary Simulations of Proteins and Their Hydration Shells by Hamiltonian Adaptive Resolution Scheme. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5647-5657.	5.3	20
6	Computational metallomics of the anticancer drug cisplatin. <i>Journal of Inorganic Biochemistry</i> , 2015, 153, 231-238.	3.5	20
7	Adaptation of Extremophilic Proteins with Temperature and Pressure: Evidence from Initiation Factor 6. <i>Journal of Physical Chemistry B</i> , 2015, 119, 7860-7873.	2.6	15
8	Structural predictions of neurobiologically relevant G-protein coupled receptors and intrinsically disordered proteins. <i>Archives of Biochemistry and Biophysics</i> , 2015, 582, 91-100.	3.0	4
9	Structural Biology of Cisplatin Complexes with Cellular Targets: The Adduct with Human Copper Chaperone Atox1 in Aqueous Solution. <i>Chemistry - A European Journal</i> , 2014, 20, 11719-11725.	3.3	14
10	Platination of the copper transporter ATP7A involved in anticancer drug resistance. <i>Dalton Transactions</i> , 2014, 43, 12085.	3.3	29
11	Conformational transition of DNA bound to Hfq probed by infrared spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 1222-1229.	2.8	34
12	From NMR Relaxation to Fractional Brownian Dynamics in Proteins: Results from a Virtual Experiment. <i>Journal of Physical Chemistry B</i> , 2011, 115, 12370-12379.	2.6	13
13	nMoldyn - Interfacing spectroscopic experiments, molecular dynamics simulations and models for time correlation functions. <i>Annales de Chimie Physique de La Soci�t� Fran�aise de La Neutronique</i> , 2011, 12, 201-232.	0.2	38
14	Fractional protein dynamics seen by nuclear magnetic resonance spectroscopy: Relating molecular dynamics simulation and experiment. <i>Journal of Chemical Physics</i> , 2010, 133, 145101.	3.0	42
15	Rigid Molecule Approximation in Memory Function-based Models for Molecular Liquids: Application to Liquid Water. <i>Zeitschrift Fur Physikalische Chemie</i> , 2009, 223, 957-978.	2.8	1
16	Relaxation dynamics of lysozyme in solution under pressure: Combining molecular dynamics simulations and quasielastic neutron scattering. <i>Chemical Physics</i> , 2008, 345, 289-297.	1.9	47
17	Scaling laws and memory effects in the dynamics of liquids and proteins. <i>Physics of Particles and Nuclei Letters</i> , 2008, 5, 189-195.	0.4	2
18	Protein dynamics from a NMR perspective: Networks of coupled rotators and fractional Brownian dynamics. <i>Journal of Chemical Physics</i> , 2008, 128, 145102.	3.0	16

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19	Influence of pressure on the slow and fast fractional relaxation dynamics in lysozyme: A simulation study. <i>Journal of Chemical Physics</i> , 2008, 128, 065102.	3.0	21
20	Estimating the influence of finite instrumental resolution on elastic neutron scattering intensities from proteins. <i>Journal of Chemical Physics</i> , 2007, 126, 125107.	3.0	21
21	Role of effective atomic masses in memory function-based models for liquids: A simulation study of liquid water. <i>Journal of Chemical Physics</i> , 2006, 125, 236102.	3.0	3
22	Pressure effect on water dynamics in tert-butyl alcohol/water solutions. <i>Journal of Physics Condensed Matter</i> , 2006, 18, S2363-S2371.	1.8	4
23	Diffusive dynamics of water in tert-butyl alcohol/water mixtures. <i>Journal of Chemical Physics</i> , 2004, 120, 4759-4767.	3.0	32
24	Water dynamics in dilute aqueous solutions of small apolar solutes by quasi-elastic neutron scattering. <i>Applied Physics A: Materials Science and Processing</i> , 2002, 74, s1339-s1341.	2.3	3
25	Conformational changes of proteins in aqueous solution induced by temperature in the pre-melting region. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 3811-3813.	2.8	14
26	Rotational and translational dynamics of lysozyme in water-glycerol solution. <i>Colloids and Surfaces B: Biointerfaces</i> , 2001, 21, 311-316.	5.0	26
27	Role of hydrophobic interactions on the stabilisation of native state of globular proteins. <i>Chemical Physics Letters</i> , 2000, 324, 344-348.	2.6	18
28	Effect of 1-alkanols on the native conformation of Lysozyme. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 4143-4146.	2.8	6
29	Effect of Trehalose on Alkaline Transition of Cytochrome-c. <i>Journal of Physical Chemistry B</i> , 2000, 104, 6889-6893.	2.6	13