

Mirco Zerbetto

List of Publications by Year in descending order

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56
papers

1,109
citations

430874

18
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414414

32
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56
all docs

56
docs citations

56
times ranked

1487
citing authors

#	ARTICLE	IF	CITATIONS
1	Parameter free evaluation of S_N2 reaction rates for halide substitution in halomethane. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 7474-7480.	2.8	0
2	Ethanol electro-oxidation reaction on the Pd(111) surface in alkaline media: insights from quantum and molecular mechanics. <i>Physical Chemistry Chemical Physics</i> , 2022, , .	2.8	2
3	Stochastic Modelling of ^{13}C NMR Spin Relaxation Experiments in Oligosaccharides. <i>Molecules</i> , 2021, 26, 2418.	3.8	1
4	Insights on the supramolecular polymorphism of poly(β -benzyl-L-glutamate) rod-like peptides from atomistic molecular dynamics simulations. <i>Journal of Materials Science</i> , 2021, 56, 16463-16474.	3.7	1
5	Conformational Entropy from Mobile Bond Vectors in Proteins: A Viewpoint that Unifies NMR Relaxation Theory and Molecular Dynamics Simulation Approaches. <i>Journal of Physical Chemistry B</i> , 2020, 124, 9323-9334.	2.6	9
6	Multiscale modeling of reaction rates: application to archetypal S_N2 nucleophilic substitutions. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 3455-3465.	2.8	4
7	Glycosidic linkage flexibility: The ϕ torsion angle has a bimodal distribution in β -D-GlcNAc-6- <i>O</i> -Me as deduced from ^{13}C NMR spin relaxation. <i>Journal of Chemical Physics</i> , 2020, 152, 035103.	3.0	9
8	DiTe2: Calculating the diffusion tensor for flexible molecules. <i>Journal of Computational Chemistry</i> , 2019, 40, 697-705.	3.3	7
9	Mesoporous Carbon with Different Density of Thiophenic-Like Functional Groups and Their Effect on Oxygen Reduction. <i>ChemSusChem</i> , 2019, 12, 4229-4239.	6.8	29
10	Local Ordering at the H Sites of the Rho GTPase Binding Domain of Plexin-B1: Impact of Dimerization. <i>Journal of Physical Chemistry B</i> , 2019, 123, 8019-8033.	2.6	6
11	Evaluating rotation diffusion properties of molecules from short trajectories. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 3662-3668.	2.8	4
12	Stochastic modeling of macromolecules in solution. I. Relaxation processes. <i>Journal of Chemical Physics</i> , 2019, 150, 184107.	3.0	11
13	Stochastic modeling of macromolecules in solution. II. Spectral densities. <i>Journal of Chemical Physics</i> , 2019, 150, 184108.	3.0	9
14	Local Ordering at Mobile Sites in Proteins: Combining Perspectives from NMR Relaxation and Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2019, 123, 2745-2755.	2.6	10
15	Effect of Different Conformational Distributions on the Ultrafast Coherence Dynamics in Porphyrin-Based Polymers. <i>Journal of Physical Chemistry C</i> , 2019, 123, 10212-10224.	3.1	10
16	Differential Dynamics at Glycosidic Linkages of an Oligosaccharide as Revealed by ^{13}C NMR Spin Relaxation and Stochastic Modeling. <i>Journal of Physical Chemistry B</i> , 2018, 122, 2287-2294.	2.6	4
17	Density Functional Theory (DFT) and Experimental Evidences of Metal-Support Interaction in Platinum Nanoparticles Supported on Nitrogen- and Sulfur-Doped Mesoporous Carbons: Synthesis, Activity, and Stability. <i>ACS Catalysis</i> , 2018, 8, 1122-1137.	11.2	83
18	Probing the correlation between Pt-support interaction and oxygen reduction reaction activity in mesoporous carbon materials modified with Pt-N active sites. <i>Electrochimica Acta</i> , 2018, 277, 287-300.	5.2	45

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19	¹⁵ N-Related Conformational Entropy Changes Entailed By Plexin-B1 RBD Dimerization: Combined Molecular Dynamics/NMR Relaxation Approach. Journal of Physical Chemistry B, 2017, 121, 3007-3015.	2.6	8
20	Integrated Computational Approach to the Electron Paramagnetic Resonance Characterization of Rigid ¹⁰ -Helical Peptides with TOAC Nitroxide Spin Labels. Journal of Physical Chemistry B, 2017, 121, 4379-4387.	2.6	4
21	Spectroscopic Insights into Carbon Dot Systems. Journal of Physical Chemistry Letters, 2017, 8, 2236-2242.	4.6	111
22	Synthesis of Gold Nanoparticles in Liquid Environment by Laser Ablation with Geometrically Confined Configurations: Insights To Improve Size Control and Productivity. Journal of Physical Chemistry C, 2016, 120, 9453-9463.	3.1	77
23	Multiscale modeling for interpreting nuclear magnetic resonance relaxation in flexible molecules. International Journal of Quantum Chemistry, 2016, 116, 1706-1722.	2.0	5
24	Loop Electrostatics Asymmetry Modulates the Preexisting Conformational Equilibrium in Thrombin. Biochemistry, 2016, 55, 3984-3994.	2.5	17
25	Flexibility at a glycosidic linkage revealed by molecular dynamics, stochastic modeling, and ¹³ C NMR spin relaxation: conformational preferences of β -D-GlcNAc(1 \rightarrow 6)-GlcNAc(1 \rightarrow 2)-Mannose. Journal of Physical Chemistry B, 2016, 18, 3086-3096.	2.8	52
26	Probing the conformational energetics of alkyl thiols on gold surfaces by means of a morphing/steering non-equilibrium tool. Physical Chemistry Chemical Physics, 2015, 17, 8038-8052.	2.8	5
27	Towards bulk thermodynamics via non-equilibrium methods: gaseous methane as a case study. Physical Chemistry Chemical Physics, 2015, 17, 1966-1979.	2.8	7
28	Multidimensional integration through Markovian sampling under steered function morphing: A physical guise from statistical mechanics. Computer Physics Communications, 2015, 195, 129-139.	7.5	1
29	Conformational Mobility in Monolayer-Protected Nanoparticles: From Torsional Free Energy Profiles to NMR Relaxation. Journal of Physical Chemistry C, 2015, 119, 20100-20110.	3.1	17
30	Summation through stochastic drawing of addends under steered morphing. Journal of Computational and Applied Mathematics, 2015, 278, 101-109.	2.0	1
31	Lifetime Shortening and Fast Energy Transfer Processes upon Dimerization of a β -Sheet-Strapped Peptide. ChemPhysChem, 2014, 15, 310-319.	2.1	0
32	Computational Study of Environmental Effects on Torsional Free Energy Surface of N-Acetyl-L-methyl-L-alanyl-L-alanine Dipeptide. Journal of Chemical Education, 2014, 91, 96-102.	2.3	11
33	Bulky toroidal and vesicular self-assembled nanostructures from fullerene end-capped rod-like polymers. Chemical Communications, 2014, 50, 4571-4574.	4.1	20
34	Photoresponsive Supramolecular Architectures Based on Polypeptide Hybrids. Macromolecules, 2014, 47, 7272-7283.	4.8	13
35	Looking for some free energy? Call JEFREE (β). Journal of Computational Chemistry, 2014, 35, 1865-1881.	3.3	12
36	Analysis of ¹⁵ N- ¹ H NMR Relaxation in Proteins by a Combined Experimental and Molecular Dynamics Simulation Approach: Picosecond-Nanosecond Dynamics of the Rho GTPase Binding Domain of Plexin-B1 in the Dimeric State Indicates Allosteric Pathways. Journal of Physical Chemistry B, 2013, 117, 174-184.	2.6	28

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37	Computational tools for the interpretation of electron spin resonance spectra in solution. <i>Molecular Physics</i> , 2013, 111, 2746-2756.	1.7	18
38	Sorting Nanoparticles by Centrifugal Fields in Clean Media. <i>Journal of Physical Chemistry C</i> , 2013, 117, 13217-13229.	3.1	83
39	Stochastic Modeling of Flexible Biomolecules Applied to NMR Relaxation. I. Internal Dynamics of Cyclodextrins: β -Cyclodextrin as a Case Study. <i>Journal of Physical Chemistry B</i> , 2012, 116, 13159-13171.	2.6	12
40	Interpretation of cw-ESR spectra of p-methyl-thio-phenyl-nitronyl nitroxide in a nematic liquid crystalline phase. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 3200.	2.8	7
41	SRLS Analysis of ^{15}N Spin Relaxation from <i>E. coli</i> Ribonuclease HI: The Tensorial Perspective. <i>Journal of Physical Chemistry B</i> , 2012, 116, 886-894.	2.6	15
42	Stochastic Modeling of Flexible Biomolecules Applied to NMR Relaxation. 2. Interpretation of Complex Dynamics in Linear Oligosaccharides. <i>Journal of Physical Chemistry B</i> , 2012, 116, 14541-14555.	2.6	19
43	<i>In Silico</i> Interpretation of cw-ESR at 9 and 95 GHz of Mono- and bis- TOAC-Labeled Aib-Homopeptides in Fluid and Frozen Acetonitrile. <i>Journal of Physical Chemistry B</i> , 2011, 115, 13026-13036.	2.6	5
44	Backbone Dynamics of Deoxy and Carbonmonoxy Hemoglobin by NMR/SRLS. <i>Journal of Physical Chemistry B</i> , 2011, 115, 143-157.	2.6	13
45	Integrated Computational Approach to the Analysis of NMR Relaxation in Proteins: Application to ps α 'ns Main Chain ^{15}N and Global Dynamics of the Rho GTPase Binding Domain of Plexin-B1. <i>Journal of Physical Chemistry B</i> , 2011, 115, 376-388.	2.6	32
46	C++OPPS, a new software for the interpretation of protein dynamics from nuclear magnetic resonance measurements. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 387-405.	2.0	9
47	Hydrodynamic modeling of diffusion tensor properties of flexible molecules. <i>Journal of Computational Chemistry</i> , 2009, 30, 2-13.	3.3	36
48	Simulation of electron spin resonance spectroscopy in diverse environments: An integrated approach. <i>Computer Physics Communications</i> , 2009, 180, 2680-2697.	7.5	20
49	An integrated approach to NMR spin relaxation in flexible biomolecules: Application to $^2\text{-D}$ -glucopyranosyl-($1\alpha'$) $^1\text{-D}$ -mannopyranosyl-OMe. <i>Journal of Chemical Physics</i> , 2009, 131, 234501.	3.0	27
50	General Theoretical/Computational Tool for Interpreting NMR Spin Relaxation in Proteins. <i>Journal of Physical Chemistry B</i> , 2009, 113, 13613-13625.	2.6	50
51	Modeling of cw-EPR Spectra of Propagating Radicals in Methacrylic Polymerization at Different Temperatures. <i>Journal of Physical Chemistry B</i> , 2008, 112, 11202-11208.	2.6	13
52	On the interpretation of continuous wave electron spin resonance spectra of tempo-palmitate in 5-cyanobiphenyl. <i>Journal of Chemical Physics</i> , 2008, 128, 024501.	3.0	20
53	Unraveling Solvent-Driven Equilibria between $^1\text{-}$ and $3\text{-}10\text{-}$ Helices through an Integrated Spin Labeling and Computational Approach. <i>Journal of the American Chemical Society</i> , 2007, 129, 11248-11258.	13.7	40
54	Ab Initio Modeling of CW-ESR Spectra of the Double Spin Labeled Peptide Fmoc-(Aib-Aib-TOAC) $_2$ -Aib-OMe in Acetonitrile. <i>Journal of Physical Chemistry B</i> , 2007, 111, 2668-2674.	2.6	32

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55	Development and Validation of an Integrated Computational Approach for the Modeling of cw-ESR Spectra of Free Radicals in Solution: Δ p-(Methylthio)phenyl Nitronyl Nitroxide in Toluene as a Case Study. <i>Journal of the American Chemical Society</i> , 2006, 128, 15865-15873.	13.7	38
56	Stochastic Modeling of CW-ESR Spectroscopy of [60]Fulleropyrrolidine Bisadducts with Nitroxide Probes. <i>Journal of the American Chemical Society</i> , 2006, 128, 4734-4741.	13.7	27