Mirco Zerbetto

List of Publications by Year
in descending order

56 papers	1,109 citations	430874 18 h-index	414414 32 g-index
56 all docs	56 docs citations	56 times ranked	1487 citing authors

#	Article	IF	Citations
1	Spectroscopic Insights into Carbon Dot Systems. Journal of Physical Chemistry Letters, 2017, 8, 2236-2242.	4.6	111
2	Sorting Nanoparticles by Centrifugal Fields in Clean Media. Journal of Physical Chemistry C, 2013, 117, 13217-13229.	3.1	83
3	Density Functional Theory (DFT) and Experimental Evidences of Metalâ€“Support Interaction in Platinum Nanoparticles Supported on Nitrogen- and Sulfur-Doped Mesoporous Carbons: Synthesis, Activity, and Stability. ACS Catalysis, 2018, 8, 1122-1137.	11.2	83
4	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
5	General Theoretical/Computational Tool for Interpreting NMR Spin Relaxation in Proteins. Journal of Physical Chemistry B, 2009, 113, 13613-13625.	2.6	50
6	Probing the correlation between Pt-support interaction and oxygen reduction reaction activity in mesoporous carbon materials modified with Pt-N active sites. Electrochimica Acta, 2018, 277, 287-300.	5.2	45
7	Unraveling Solvent-Driven Equilibria between Î±- and 3₁₀-Helices through an Integrated Spin Labeling and Computational Approach. Journal of the American Chemical Society, 2007, 129, 11248-11258.	13.7	40
8	Development and Validation of an Integrated Computational Approach for the Modeling of cw-ESR Spectra of Free Radicals in Solution:Âp-(Methylthio)phenyl Nitronylnitroxide in Toluene as a Case Study. Journal of the American Chemical Society, 2006, 128, 15865-15873.	13.7	38
9	Hydrodynamic modeling of diffusion tensor properties of flexible molecules. Journal of Computational Chemistry, 2009, 30, 2-13.	3.3	36
10	Ab InitioModeling of CW-ESR Spectra of the Double Spin Labeled Peptide Fmoc-(Aib-Aib-TOAC)2-Aib-OMe in Acetonitrile. Journal of Physical Chemistry B, 2007, 111, 2668-2674.	2.6	32
11	Integrated Computational Approach to the Analysis of NMR Relaxation in Proteins: Application to psâ^ns Main Chain ¹⁵Nâ^’¹H and Global Dynamics of the Rho GTPase Binding Domain of Plexin-B1. Journal of Physical Chemistry B, 2011, 115, 376-388.	2.6	32
12	Mesoporous Carbon with Different Density of Thiophenicâ€Like Functional Groups and Their Effect on Oxygen Reduction. ChemSusChem, 2019, 12, 4229-4239.	6.8	29
13	Analysis of ¹⁵Nâ€“¹H NMR Relaxation in Proteins by a Combined Experimental and Molecular Dynamics Simulation Approach: Picosecondâ€“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
14	Stochastic Modeling of CW-ESR Spectroscopy of [60]Fulleropyrrolidine Bisadducts with Nitroxide Probes. Journal of the American Chemical Society, 2006, 128, 4734-4741.	13.7	27
15	An integrated approach to NMR spin relaxation in flexible biomolecules: Application to Î²-D-glucopyranosyl-(1â†’6)-Î±-D-mannopyranosyl-OMe. Journal of Chemical Physics, 2009, 131, 234501.	3.0	27
16	On the interpretation of continuous wave electron spin resonance spectra of tempo-palmitate in 5-cyanobiphenyl. Journal of Chemical Physics, 2008, 128, 024501.	3.0	20
17	Simulation of electron spin resonance spectroscopy in diverse environments: An integrated approach. Computer Physics Communications, 2009, 180, 2680-2697.	7.5	20
18	Bulky toroidal and vesicular self-assembled nanostructures from fullerene end-capped rod-like polymers. Chemical Communications, 2014, 50, 4571-4574.	4.1	20

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19	Stochastic Modeling of Flexible Biomolecules Applied to NMR Relaxation. 2. Interpretation of Complex Dynamics in Linear Oligosaccharides. Journal of Physical Chemistry B, 2012, 116, 14541-14555.	2.6	19
20	Computational tools for the interpretation of electron spin resonance spectra in solution. Molecular Physics, 2013, 111, 2746-2756.	1.7	18
21	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
22	Loop Electrostatics Asymmetry Modulates the Preexisting Conformational Equilibrium in Thrombin. Biochemistry, 2016, 55, 3984-3994.	2.5	17
23	SRLS Analysis of ¹⁵N Spin Relaxation from E. coli Ribonuclease HI: The Tensorial Perspective. Journal of Physical Chemistry B, 2012, 116, 886-894.	2.6	15
24	Modeling of cw-EPR Spectra of Propagating Radicals in Methacrylic Polymerization at Different Temperatures. Journal of Physical Chemistry B, 2008, 112, 11202-11208.	2.6	13
25	Backbone Dynamics of Deoxy and Carbonmonoxy Hemoglobin by NMR/SRLS. Journal of Physical Chemistry B, 2011, 115, 143-157.	2.6	13
26	Photoresponsive Supramolecular Architectures Based on Polypeptide Hybrids. Macromolecules, 2014, 47, 7272-7283.	4.8	13
27	Stochastic Modeling of Flexible Biomolecules Applied to NMR Relaxation. I. Internal Dynamics of Cyclodextrins: Î³-Cyclodextrin as a Case Study. Journal of Physical Chemistry B, 2012, 116, 13159-13171.	2.6	12
28	Looking for some free energy? Call JEFREE (â€¦). Journal of Computational Chemistry, 2014, 35, 1865-1881.	3.3	12
29	Flexibility at a glycosidic linkage revealed by molecular dynamics, stochastic modeling, and ¹³C NMR spin relaxation: conformational preferences of Î±-<scp>l</scp>-Rhap-Î±-(1 â†') Tj ETQq1 1 0.784314 rgBT /Ove Physics, 2016, 18, 3086-3096.	2.8	12
30	Computational Study of Environmental Effects on Torsional Free Energy Surface of N-Acetyl-Nâ€²-methyl-l-alanylamide Dipeptide. Journal of Chemical Education, 2014, 91, 96-102.	2.3	11
31	Stochastic modeling of macromolecules in solution. I. Relaxation processes. Journal of Chemical Physics, 2019, 150, 184107.	3.0	11
32	Local Ordering at Mobile Sites in Proteins: Combining Perspectives from NMR Relaxation and Molecular Dynamics. Journal of Physical Chemistry B, 2019, 123, 2745-2755.	2.6	10
33	Effect of Different Conformational Distributions on the Ultrafast Coherence Dynamics in Porphyrin-Based Polymers. Journal of Physical Chemistry C, 2019, 123, 10212-10224.	3.1	10
34	C++OPPS, a new software for the interpretation of protein dynamics from nuclear magnetic resonance measurements. International Journal of Quantum Chemistry, 2010, 110, 387-405.	2.0	9
35	Stochastic modeling of macromolecules in solution. II. Spectral densities. Journal of Chemical Physics, 2019, 150, 184108.	3.0	9
36	Conformational Entropy from Mobile Bond Vectors in Proteins: A Viewpoint that Unifies NMR Relaxation Theory and Molecular Dynamics Simulation Approaches. Journal of Physical Chemistry B, 2020, 124, 9323-9334.	2.6	9

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37	Glycosidic linkage flexibility: The Ï‘ torsion angle has a bimodal distribution in Î±-L-Rhap-(1â†’2)-Î±-L-Rhap-OMe as deduced from 13C NMR spin relaxation. Journal of Chemical Physics, 2020, 152, 035103.	3.0	9
38	¹⁵Nâ€“H-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
39	Interpretation of cw-ESR spectra of p-methyl-thio-phenyl-nitronyl nitroxide in a nematic liquid crystalline phase. Physical Chemistry Chemical Physics, 2012, 14, 3200.	2.8	7
40	Towards bulk thermodynamics via non-equilibrium methods: gaseous methane as a case study. Physical Chemistry Chemical Physics, 2015, 17, 1966-1979.	2.8	7
41	DiTe2: Calculating the diffusion tensor for flexible molecules. Journal of Computational Chemistry, 2019, 40, 697-705.	3.3	7
42	Local Ordering at the Nâ€“H Sites of the Rho GTPase Binding Domain of Plexin-B1: Impact of Dimerization. Journal of Physical Chemistry B, 2019, 123, 8019-8033.	2.6	6
43	In Silico Interpretation of cw-ESR at 9 and 95 GHz of Mono- and bis- TOAC-Labeled Aib-Homopeptides in Fluid and Frozen Acetonitrile. Journal of Physical Chemistry B, 2011, 115, 13026-13036.	2.6	5
44	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
45	Multiscale modeling for interpreting nuclear magnetic resonance relaxation in flexible molecules. International Journal of Quantum Chemistry, 2016, 116, 1706-1722.	2.0	5
46	Integrated Computational Approach to the Electron Paramagnetic Resonance Characterization of Rigid 3₁₀-Helical Peptides with TOAC Nitroxide Spin Labels. Journal of Physical Chemistry B, 2017, 121, 4379-4387.	2.6	4
47	Differential Dynamics at Glycosidic Linkages of an Oligosaccharide as Revealed by ¹³C NMR Spin Relaxation and Stochastic Modeling. Journal of Physical Chemistry B, 2018, 122, 2287-2294.	2.6	4
48	Evaluating rotation diffusion properties of molecules from short trajectories. Physical Chemistry Chemical Physics, 2019, 21, 3662-3668.	2.8	4
49	Multiscale modeling of reaction rates: application to archetypal SN2 nucleophilic substitutions. Physical Chemistry Chemical Physics, 2020, 22, 3455-3465.	2.8	4
50	Ethanol electro-oxidation reaction on the Pd(111) surface in alkaline media: insights from quantum and molecular mechanics. Physical Chemistry Chemical Physics, 2022, , .	2.8	2
51	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
52	Summation through stochastic drawing of addends under steered morphing. Journal of Computational and Applied Mathematics, 2015, 278, 101-109.	2.0	1
53	Stochastic Modelling of 13C NMR Spin Relaxation Experiments in Oligosaccharides. Molecules, 2021, 26, 2418.	3.8	1
54	Insights on the supramolecular polymorphism of poly(Î³-benzyl-L-glutamate) rod-like peptides from atomistic molecular dynamics simulations. Journal of Materials Science, 2021, 56, 16463-16474.	3.7	1

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55	Lifetime Shortening and Fast Energyâ€Transfer Processes upon Dimerization of a Aâ€Ïâ€Dâ€Ïâ€A Molecule. ChemPhysChem, 2014, 15, 310-319.	2.1	0
56	Parameter free evaluation of S_N2 reaction rates for halide substitution in halomethane. Physical Chemistry Chemical Physics, 2022, 24, 7474-7480.	2.8	0