Antonino Polimeno

List of Publications by Year
in descending order

78 papers	1,883 citations	279798 23 h-index	289244 40 g-index
80 all docs	80 docs citations	80 times ranked	1171 citing authors

#	Article	IF	Citations
1	Parameter free evaluation of S_N2 reaction rates for halide substitution in halomethane. Physical Chemistry Chemical Physics, 2022, 24, 7474-7480.	2.8	0
2	Enabling Circular Economy: The Overlooked Role of Inorganic Materials Chemistry. Chemistry - A European Journal, 2021, 27, 6676-6695.	3.3	6
3	Stochastic Modelling of 13C NMR Spin Relaxation Experiments in Oligosaccharides. Molecules, 2021, 26, 2418.	3.8	1
4	Modelling of Ca²⁺-promoted structural effects in wild type and post-translationally modified Connexin26. Molecular Simulation, 2020, 46, 235-245.	2.0	0
5	Multiscale modeling of reaction rates: application to archetypal SN2 nucleophilic substitutions. Physical Chemistry Chemical Physics, 2020, 22, 3455-3465.	2.8	4
6	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
7	DiTe2: Calculating the diffusion tensor for flexible molecules. Journal of Computational Chemistry, 2019, 40, 697-705.	3.3	7
8	Similarity and Specificity of Chlorophyll b Triplet State in Comparison to Chlorophyll a as Revealed by EPR/ENDOR and DFT Calculations. Journal of Physical Chemistry B, 2019, 123, 8232-8239.	2.6	8
9	Evaluating rotation diffusion properties of molecules from short trajectories. Physical Chemistry Chemical Physics, 2019, 21, 3662-3668.	2.8	4
10	Stochastic modeling of macromolecules in solution. I. Relaxation processes. Journal of Chemical Physics, 2019, 150, 184107.	3.0	11
11	Stochastic modeling of macromolecules in solution. II. Spectral densities. Journal of Chemical Physics, 2019, 150, 184108.	3.0	9
12	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
13	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
14	Decomposition of Proteins into Dynamic Units from Atomic Cross-Correlation Functions. Journal of Chemical Theory and Computation, 2017, 13, 309-319.	5.3	11
15	Multiscale modeling for interpreting nuclear magnetic resonance relaxation in flexible molecules. International Journal of Quantum Chemistry, 2016, 116, 1706-1722.	2.0	5
16	General AMBER Force Field Parameters for Diphenyl Diselenides and Diphenyl Ditellurides. Journal of Physical Chemistry A, 2016, 120, 4389-4400.	2.5	22
17	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
18	Selenocysteine oxidation in glutathione peroxidase catalysis: an MS-supported quantum mechanics study. Free Radical Biology and Medicine, 2015, 87, 1-14.	2.9	100

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19	Evidence for water-mediated tripletâ€“triplet energy transfer in the photoprotective site of the peridininâ€“chlorophyll aâ€“protein. Biochimica Et Biophysica Acta - Bioenergetics, 2014, 1837, 85-97.	1.0	27
20	On the reliability of NMR relaxation data analyses: A Markov Chain Monte Carlo approach. Journal of Magnetic Resonance, 2014, 246, 94-103.	2.1	8
21	Role of gamma carboxylated Glu47 in connexin 26 hemichannel regulation by extracellular Ca2+: Insight from a local quantum chemistry study. Biochemical and Biophysical Research Communications, 2014, 445, 10-15.	2.1	17
22	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
23	Computational tools for the interpretation of electron spin resonance spectra in solution. Molecular Physics, 2013, 111, 2746-2756.	1.7	18
24	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
25	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
26	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
27	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
28	Heuristic approaches to the optimization of acceptor systems in bulk heterojunction cells: a computational study. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	2
29	Methyl Dynamics of a Ca²⁺â^'Calmodulinâ^'Peptide Complex from NMR/SRLS. Journal of Physical Chemistry B, 2011, 115, 354-365.	2.6	15
30	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
31	Backbone Dynamics of Deoxy and Carbonmonoxy Hemoglobin by NMR/SRLS. Journal of Physical Chemistry B, 2011, 115, 143-157.	2.6	13
32	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
33	Time correlated fluorescence characterization of an asymmetrically focused flow in a microfluidic device. Microfluidics and Nanofluidics, 2011, 10, 551-561.	2.2	10
34	Strategy for the improvement of mixing in microdevices. Houille Blanche, 2011, 97, 79-85.	0.3	0
35	Structural dynamics of bio-macromolecules by NMR: The slowly relaxing local structure approach. Progress in Nuclear Magnetic Resonance Spectroscopy, 2010, 56, 360-405.	7.5	86
36	Interpretation of the emission fluorescence spectra of two fluoroionophores: DMABNâ€Crown4 and DMABNâ€Crown5. International Journal of Quantum Chemistry, 2010, 110, 368-375.	2.0	1

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37	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
38	Comment on â€œThe physical basis of model-free analysis of NMR relaxation data from proteins and complex fluidsâ€•[J. Chem. Phys. 131, 224507 (2009)]. Journal of Chemical Physics, 2010, 132, 207101.	3.0	11
39	Time-Evolution Equations for Particle Dispersions in Nematic Liquid Crystal Media. Molecular Crystals and Liquid Crystals, 2010, 516, 167-173.	0.9	0
40	Hydrodynamic modeling of diffusion tensor properties of flexible molecules. Journal of Computational Chemistry, 2009, 30, 2-13.	3.3	36
41	Simulation of electron spin resonance spectroscopy in diverse environments: An integrated approach. Computer Physics Communications, 2009, 180, 2680-2697.	7.5	20
42	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
43	General Theoretical/Computational Tool for Interpreting NMR Spin Relaxation in Proteins. Journal of Physical Chemistry B, 2009, 113, 13613-13625.	2.6	50
44	Evaluation of translational friction coefficients of micro-sized spherical probes in nematic liquid crystals. Theoretical Chemistry Accounts, 2008, 120, 591-597.	1.4	0
45	An integrated approach for the interpretation of emission fluorescence of DMABN-Crown derivatives in polar environments. Chemical Physics Letters, 2008, 467, 204-209.	2.6	2
46	Integrated Approach for Modeling the Emission Fluorescence of 4-(N,N-Dimethylamino)benzonitrile in Polar Environments. Journal of Physical Chemistry B, 2008, 112, 8106-8113.	2.6	15
47	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
48	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
49	Integrated computational strategies for UV/vis spectra of large molecules in solution. Chemical Society Reviews, 2007, 36, 1724.	38.1	162
50	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
51	An Improved Picture of Methyl Dynamics in Proteins from Slowly Relaxing Local Structure Analysis of ²H Spin Relaxation. Journal of Physical Chemistry B, 2007, 111, 12865-12875.	2.6	23
52	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
53	A Many-Body Stochastic Approach to Rotational Motions in Liquids. Advances in Chemical Physics, 2007, , 89-206.	0.3	59
54	Methyl Dynamics in Proteins from NMR Slowly Relaxing Local Structure Spin Relaxation Analysis:Â A New Perspective. Journal of Physical Chemistry B, 2006, 110, 20615-20628.	2.6	22

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55	Toward an integrated computational approach to CW-ESR spectra of free radicals. Physical Chemistry Chemical Physics, 2006, 8, 4609.	2.8	73
56	Protein Dynamics from NMR:Â The Slowly Relaxing Local Structure Analysis Compared with Model-Free Analysisâ€. Journal of Physical Chemistry A, 2006, 110, 8366-8396.	2.5	82
57	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
58	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
59	Evaluation of the viscoelastic properties of a nematic dimer by cone-and-plate rheo-nuclear magnetic resonance spectroscopy and comparison with Leslieâ€“Ericksen theory. Journal of Chemical Physics, 2002, 117, 4550-4556.	3.0	12
60	Simulations of Flow-Induced Director Patterns in Nematic Liquid Crystals Through Leslie-Ericksen Equations in Two Dimensions. Molecular Crystals and Liquid Crystals, 2000, 351, 135-143.	0.3	4
61	Nematodynamics Equations in Two Dimensions. Molecular Crystals and Liquid Crystals, 1999, 336, 17-32.	0.3	7
62	Flow Patterns of the Nematic Director in a Rotating Cylindrical Sample. Molecular Crystals and Liquid Crystals, 1999, 328, 541-548.	0.3	5
63	Two-dimensional hydrodynamical description of a rotating nematic sample in a magnetic field. Liquid Crystals, 1998, 25, 545-552.	2.2	14
64	A 250 GHz ESR study of o-terphenyl: Dynamic cage effects above Tc. Journal of Chemical Physics, 1997, 106, 9996-10015.	3.0	73
65	A stochastic cage model for linear solutes. Journal of Chemical Physics, 1997, 107, 7884-7893.	3.0	22
66	Rotational dynamics of axially symmetric solutes in isotropic solvents. II. The stochastic model. Journal of Chemical Physics, 1996, 104, 1090-1104.	3.0	31
67	Studies of spin relaxation and molecular dynamics in liquid crystals by twoâ€dimensional Fourier transform electron spin resonance. II. Perdeuteratedâ€tempone in butoxy benzylidene octylaniline and dynamic cage effects. Journal of Chemical Physics, 1996, 105, 5773-5791.	3.0	28
68	Studies of spin relaxation and molecular dynamics in liquid crystals by twoâ€dimensional Fourier transform electron spin resonance. I. Cholestane in butoxy benzylideneâ€octylaniline and dynamic cage effects. Journal of Chemical Physics, 1996, 105, 5753-5772.	3.0	34
69	Numerical test of Kramers reaction rate theory in two dimensions. Journal of Chemical Physics, 1996, 105, 6342-6357.	3.0	20
70	Simulated Time Resolved Fluorescence in Ordered Phases. Molecular Crystals and Liquid Crystals, 1996, 290, 163-172.	0.3	1
71	Rotational dynamics of axially symmetric solutes in isotropic liquids. I. A collective cage description from molecular dynamics simulations. Journal of Chemical Physics, 1995, 102, 8094-8106.	3.0	29
72	Slow Motional ESR in Complex Fluids: The Slowly Relaxing Local Structure Model of Solvent Cage Effects. The Journal of Physical Chemistry, 1995, 99, 10995-11006.	2.9	176

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73	A cage model of liquids supported by molecular dynamics simulations. II. The stochastic model. Journal of Chemical Physics, 1994, 101, 703-712.	3.0	18
74	A cage model of liquids supported by molecular dynamics simulations. I. The cage variables. Journal of Chemical Physics, 1994, 101, 693-702.	3.0	22
75	Stochastic Model for Solvent-Assisted Intramolecular Charge-Transfer. The Journal of Physical Chemistry, 1994, 98, 12158-12168.	2.9	42
76	Diffusion model for a reactive coordinate coupled to a solvent variable of different timescale. Molecular Physics, 1992, 75, 1203-1216.	1.7	12
77	Approximate and numerically exact solutions of the Fokker-Planck equation with bistable potentials. Chemical Physics, 1989, 131, 281-293.	1.9	17
78	Conformational processes and cooperativity effects in chain molecules. Chemical Physics Letters, 1988, 151, 531-536.	2.6	14