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	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
2	Integrated computational strategies for UV/vis spectra of large molecules in solution. Chemical Society Reviews, 2007, 36, 1724.	38.1	162
3	Selenocysteine oxidation in glutathione peroxidase catalysis: an MS-supported quantum mechanics study. Free Radical Biology and Medicine, 2015, 87, 1-14.	2.9	100
4	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
5	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
6	A 250 GHz ESR study of o-terphenyl: Dynamic cage effects above Tc. Journal of Chemical Physics, 1997, 106, 9996-10015.	3.0	73
7	Toward an integrated computational approach to CW-ESR spectra of free radicals. Physical Chemistry Chemical Physics, 2006, 8, 4609.	2.8	73
8	A Many-Body Stochastic Approach to Rotational Motions in Liquids. Advances in Chemical Physics, 2007, , 89-206.	0.3	59
9	General Theoretical/Computational Tool for Interpreting NMR Spin Relaxation in Proteins. Journal of Physical Chemistry B, 2009, 113, 13613-13625.	2.6	50
10	Stochastic Model for Solvent-Assisted Intramolecular Charge-Transfer. The Journal of Physical Chemistry, 1994, 98, 12158-12168.	2.9	42
11	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
12	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
13	Hydrodynamic modeling of diffusion tensor properties of flexible molecules. Journal of Computational Chemistry, 2009, 30, 2-13.	3.3	36
14	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
15	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
16	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
17	Rotational dynamics of axially symmetric solutes in isotropic solvents. II. The stochastic model. Journal of Chemical Physics, 1996, 104, 1090-1104.	3.0	31
18	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

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19	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
20	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
21	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
22	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
23	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
24	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
25	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
26	A stochastic cage model for linear solutes. Journal of Chemical Physics, 1997, 107, 7884-7893.	3.0	22
27	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
28	General AMBER Force Field Parameters for Diphenyl Diselenides and Diphenyl Ditellurides. Journal of Physical Chemistry A, 2016, 120, 4389-4400.	2.5	22
29	Numerical test of Kramers reaction rate theory in two dimensions. Journal of Chemical Physics, 1996, 105, 6342-6357.	3.0	20
30	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
31	Simulation of electron spin resonance spectroscopy in diverse environments: An integrated approach. Computer Physics Communications, 2009, 180, 2680-2697.	7.5	20
32	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
33	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
34	Computational tools for the interpretation of electron spin resonance spectra in solution. Molecular Physics, 2013, 111, 2746-2756.	1.7	18
35	Approximate and numerically exact solutions of the Fokker-Planck equation with bistable potentials. Chemical Physics, 1989, 131, 281-293.	1.9	17
36	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

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37	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
38	Methyl Dynamics of a Ca²⁺â^'Calmodulinâ^'Peptide Complex from NMR/SRLS. Journal of Physical Chemistry B, 2011, 115, 354-365.	2.6	15
39	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
40	Conformational processes and cooperativity effects in chain molecules. Chemical Physics Letters, 1988, 151, 531-536.	2.6	14
41	Two-dimensional hydrodynamical description of a rotating nematic sample in a magnetic field. Liquid Crystals, 1998, 25, 545-552.	2.2	14
42	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
43	Backbone Dynamics of Deoxy and Carbonmonoxy Hemoglobin by NMR/SRLS. Journal of Physical Chemistry B, 2011, 115, 143-157.	2.6	13
44	Diffusion model for a reactive coordinate coupled to a solvent variable of different timescale. Molecular Physics, 1992, 75, 1203-1216.	1.7	12
45	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
46	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
47	Flexibility at a glycosidic linkage revealed by molecular dynamics, stochastic modeling, and ¹³C NMR spin relaxation: conformational preferences of Îł-<scp>l</scp>-Rhap-Îł-(1 â†') Tj ETQq1 1 0.784314 rgBT /Ove Physics, 2016, 18, 3086-3096.	2.8	12
48	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
49	Decomposition of Proteins into Dynamic Units from Atomic Cross-Correlation Functions. Journal of Chemical Theory and Computation, 2017, 13, 309-319.	5.3	11
50	Stochastic modeling of macromolecules in solution. I. Relaxation processes. Journal of Chemical Physics, 2019, 150, 184107.	3.0	11
51	Time correlated fluorescence characterization of an asymmetrically focused flow in a microfluidic device. Microfluidics and Nanofluidics, 2011, 10, 551-561.	2.2	10
52	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
53	Stochastic modeling of macromolecules in solution. II. Spectral densities. Journal of Chemical Physics, 2019, 150, 184108.	3.0	9
54	Glycosidic linkage flexibility: The Ïˆ torsion angle has a bimodal distribution in Îł-L-Rhap-(1â†'2)-Îł-L-Rhap-OMe as deduced from 13C NMR spin relaxation. Journal of Chemical Physics, 2020, 152, 035103.	3.0	9

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55	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
56	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
57	Nematodynamics Equations in Two Dimensions. Molecular Crystals and Liquid Crystals, 1999, 336, 17-32.	0.3	7
58	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
59	DiTe2: Calculating the diffusion tensor for flexible molecules. Journal of Computational Chemistry, 2019, 40, 697-705.	3.3	7
60	Enabling Circular Economy: The Overlooked Role of Inorganic Materials Chemistry. Chemistry - A European Journal, 2021, 27, 6676-6695.	3.3	6
61	Flow Patterns of the Nematic Director in a Rotating Cylindrical Sample. Molecular Crystals and Liquid Crystals, 1999, 328, 541-548.	0.3	5
62	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
63	Multiscale modeling for interpreting nuclear magnetic resonance relaxation in flexible molecules. International Journal of Quantum Chemistry, 2016, 116, 1706-1722.	2.0	5
64	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
65	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
66	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
67	Evaluating rotation diffusion properties of molecules from short trajectories. Physical Chemistry Chemical Physics, 2019, 21, 3662-3668.	2.8	4
68	Multiscale modeling of reaction rates: application to archetypal SN2 nucleophilic substitutions. Physical Chemistry Chemical Physics, 2020, 22, 3455-3465.	2.8	4
69	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
70	Heuristic approaches to the optimization of acceptor systems in bulk heterojunction cells: a computational study. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	2
71	Simulated Time Resolved Fluorescence in Ordered Phases. Molecular Crystals and Liquid Crystals, 1996, 290, 163-172.	0.3	1
72	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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73	Stochastic Modelling of 13C NMR Spin Relaxation Experiments in Oligosaccharides. Molecules, 2021, 26, 2418.	3.8	1
74	Evaluation of translational friction coefficients of micro-sized spherical probes in nematic liquid crystals. Theoretical Chemistry Accounts, 2008, 120, 591-597.	1.4	0
75	Time-Evolution Equations for Particle Dispersions in Nematic Liquid Crystal Media. Molecular Crystals and Liquid Crystals, 2010, 516, 167-173.	0.9	0
76	Modelling of Ca²⁺-promoted structural effects in wild type and post-translationally modified Connexin26. Molecular Simulation, 2020, 46, 235-245.	2.0	0
77	Strategy for the improvement of mixing in microdevices. Houille Blanche, 2011, 97, 79-85.	0.3	0
78	Parameter free evaluation of S_N2 reaction rates for halide substitution in halomethane. Physical Chemistry Chemical Physics, 2022, 24, 7474-7480.	2.8	0