

Giovanni La Penna

List of Publications by Year in descending order

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84
papers

1,585
citations

331670

21
h-index

345221

36
g-index

88
all docs

88
docs citations

88
times ranked

1697
citing authors

#	ARTICLE	IF	CITATIONS
1	Aggregates Sealed by Ions. <i>Methods in Molecular Biology</i> , 2022, 2340, 309-341.	0.9	3
2	Modelling Protein Plasticity: The Example of Frataxin and Its Variants. <i>Molecules</i> , 2022, 27, 1955.	3.8	2
3	Implementations of replica-permutation and replica sub-permutation methods into LAMMPS. <i>Computer Physics Communications</i> , 2022, 276, 108362.	7.5	2
4	Amyloid β Dodecamer Disrupts the Neuronal Membrane More Strongly than the Mature Fibril: Understanding the Role of Oligomers in Neurotoxicity. <i>Journal of Physical Chemistry B</i> , 2022, 126, 3659-3672.	2.6	9
5	Polyphenols as Potential Metal Chelation Compounds Against Alzheimer's Disease. <i>Journal of Alzheimer's Disease</i> , 2021, 82, S335-S357.	2.6	65
6	Cu(II)-Glycerol-N-Ethylmorpholine Complex Stability Revealed by X-ray Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2021, 125, 1483-1492.	3.1	3
7	Probing the Structure of Toxic Amyloid- β Oligomers with Electron Spin Resonance and Molecular Modeling. <i>ACS Chemical Neuroscience</i> , 2021, 12, 1150-1161.	3.5	9
8	Measuring Shared Electrons in Extended Molecular Systems: Covalent Bonds from Plane-Wave Representation of Wave Function. <i>Molecules</i> , 2021, 26, 4044.	3.8	1
9	Zn-Induced Interactions Between SARS-CoV-2 orf7a and BST2/Tetherin. <i>ChemistryOpen</i> , 2021, 10, 1133-1141.	1.9	11
10	SARS-CoV-2 Virion Stabilization by Zn Binding. <i>Frontiers in Molecular Biosciences</i> , 2020, 7, 222.	3.5	14
11	Emergence of Barrel Motif in Amyloid- β Trimer: A Computational Study. <i>Journal of Physical Chemistry B</i> , 2020, 124, 10617-10631.	2.6	12
12	Nanosopic insights into the surface conformation of neurotoxic amyloid β oligomers. <i>RSC Advances</i> , 2020, 10, 21907-21913.	3.6	19
13	Computational Model to Unravel the Function of Amyloid- β Peptides in Contact with a Phospholipid Membrane. <i>Journal of Physical Chemistry B</i> , 2020, 124, 3300-3314.	2.6	7
14	Dealing with Cu reduction in X-ray absorption spectroscopy experiments. <i>Metallomics</i> , 2019, 11, 1401-1410.	2.4	11
15	Computational models explain how copper binding to amyloid- β peptide oligomers enhances oxidative pathways. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 8774-8784.	2.8	15
16	When Water Plays an Active Role in Electronic Structure. Insights from First-Principles Molecular Dynamics Simulations of Biological Systems. <i>Springer Series on Bio- and Neurosystems</i> , 2019, , 715-753.	0.2	0
17	Towards High-Throughput Modelling of Copper Reactivity Induced by Structural Disorder in Amyloid Peptides. <i>Chemistry - A European Journal</i> , 2018, 24, 5259-5270.	3.3	14
18	Understanding the Exceptional Properties of Nitroacetamides in Water: A Computational Model Including the Solvent. <i>Molecules</i> , 2018, 23, 3308.	3.8	3

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19	Multi-scale theoretical approach to X-ray absorption spectra in disordered systems: an application to the study of Zn(ii) in water. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 24775-24782.	2.8	10
20	Copper Binding Induces Polymorphism in Amyloid- β^2 Peptide: Results of Computational Models. <i>Journal of Physical Chemistry B</i> , 2018, 122, 7243-7252.	2.6	17
21	Structural Insights into the Osteopontin-Aptamer Complex by Molecular Dynamics Simulations. <i>Frontiers in Chemistry</i> , 2018, 6, 2.	3.6	16
22	Free Superoxide is an Intermediate in the Production of H_2O_2 by Copper(I)- β Peptide and O_2 . <i>Angewandte Chemie</i> , 2016, 128, 1097-1101.	2.0	18
23	Free Superoxide is an Intermediate in the Production of H_2O_2 by Copper(I)- β Peptide and O_2 . <i>Angewandte Chemie - International Edition</i> , 2016, 55, 1085-1089.	13.8	95
24	Modeling ^{15}N NMR chemical shift changes in protein backbone with pressure. <i>Journal of Chemical Physics</i> , 2016, 145, 085104.	3.0	7
25	Impact of Cu(II) Binding on Structures and Dynamics of β Monomer and Dimer: Molecular Dynamics Study. <i>ACS Chemical Neuroscience</i> , 2016, 7, 1348-1363.	3.5	62
26	A first-principle calculation of the XANES spectrum of Cu^{2+} in water. <i>Journal of Chemical Physics</i> , 2015, 143, 124508.	3.0	24
27	Learning chemistry with multiple first-principles simulations. <i>Molecular Simulation</i> , 2015, 41, 780-787.	2.0	3
28	Dioxygen activation in the Cu-amyloid β^2 complex. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 27270-27274.	2.8	24
29	A Cu-amyloid β^2 complex activating Fenton chemistry in Alzheimer's disease: Learning with multiple first-principles simulations. <i>AIP Conference Proceedings</i> , 2014, , .	0.4	4
30	When Water Plays an Active Role in Electronic Structure: Insights from First-Principles Molecular Dynamics Simulations of Biological Systems. <i>Springer Series in Bio-/neuroinformatics</i> , 2014, , 685-710.	0.1	0
31	Metal Ions and Intrinsically Disordered Proteins and Peptides: From Cu/Zn Amyloid- β^2 to General Principles. <i>Accounts of Chemical Research</i> , 2014, 47, 2252-2259.	15.6	221
32	Combined EPR and Molecular Modeling Study of PPI Dendrimers Interacting with Copper Ions: Effect of Generation and Maltose Decoration. <i>Journal of Physical Chemistry B</i> , 2014, 118, 12098-12111.	2.6	7
33	Coordination of Metal Ions to β^2 -Amyloid Peptide: Impact on Alzheimer's Disease. <i>Molecular Medicine and Medicinal</i> , 2013, , 127-155.	0.4	0
34	Identifying, By First-Principles Simulations, $Cu[\beta^2]$ Species Making Fenton-Type Reactions in Alzheimer's Disease. <i>Journal of Physical Chemistry B</i> , 2013, 117, 16455-16467.	2.6	51
35	Zn induced structural aggregation patterns of β^2 -amyloid peptides by first-principle simulations and XAS measurements. <i>Metallomics</i> , 2012, 4, 156-165.	2.4	33
36	Metal ions and protons compete for ligand atoms in disordered peptides: Examples from computer simulations of copper binding to the prion tandem repeat. <i>Coordination Chemistry Reviews</i> , 2012, 256, 2234-2244.	18.8	11

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37	Modeling Copper Binding to the Amyloid- β^2 Peptide at Different pH: Toward a Molecular Mechanism for Cu Reduction. <i>Journal of Physical Chemistry B</i> , 2012, 116, 11899-11910.	2.6	37
38	Insights into the Mechanisms of Amyloid Formation of Zn ^{II} -Ab11-28: pH-Dependent Zinc Coordination and Overall Charge as Key Parameters for Kinetics and the Structure of Zn ^{II} -Ab11-28 Aggregates. <i>Inorganic Chemistry</i> , 2012, 51, 7897-7902.	4.0	10
39	The mechanism of hydrogen uptake in [NiFe] hydrogenase: first-principles molecular dynamics investigation of a model compound. <i>Journal of Biological Inorganic Chemistry</i> , 2012, 17, 149-164.	2.6	3
40	Exploring the Reactions of β^2 -Amyloid ($A\beta^2$) Peptide 1-28 with Al ^{III} and Fe ^{III} Ions. <i>Inorganic Chemistry</i> , 2011, 50, 6865-6867.	4.0	42
41	Measuring electron sharing between atoms in first-principle simulations. <i>Theoretical Chemistry Accounts</i> , 2011, 130, 27-36.	1.4	6
42	Wrapped-Around Models for the Lac Operon Complex. <i>Biophysical Journal</i> , 2010, 98, 2964-2973.	0.5	9
43	Modeling the Cu ⁺ Binding in the 1-16 Region of the Amyloid- β^2 Peptide Involved in Alzheimer's Disease. <i>Journal of Physical Chemistry B</i> , 2010, 114, 15119-15133.	2.6	63
44	Modeling the interplay of glycine protonation and multiple histidine binding of copper in the prion protein octarepeat subdomains. <i>Journal of Biological Inorganic Chemistry</i> , 2009, 14, 361-374.	2.6	27
45	Modeling of the Zn ²⁺ binding in the 1-16 region of the amyloid β^2 peptide involved in Alzheimer's disease. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 6468.	2.8	31
46	Modeling the Free Energy of Polypeptides in Different Environments. <i>Macromolecules</i> , 2008, 41, 2938-2948.	4.8	9
47	Ab Initio Molecular Dynamics of Heme in Cytochrome c. <i>Journal of Physical Chemistry B</i> , 2007, 111, 1157-1164.	2.6	7
48	Anisotropic Internucleosome Interactions and Geometrical Constraints in the Organization of Chromatin. <i>Macromolecules</i> , 2007, 40, 9603-9613.	4.8	7
49	Generalized electrostatic model of the wrapping of DNA around oppositely charged proteins. <i>Biopolymers</i> , 2007, 86, 127-135.	2.4	27
50	Studying the Cu binding sites in the PrP N-terminal region: a test case for ab initio simulations. <i>European Biophysics Journal</i> , 2007, 36, 841-845.	2.2	9
51	Molecular statistics of cytochrome c: structural plasticity and molecular environment. <i>Journal of Biological Inorganic Chemistry</i> , 2007, 12, 180-193.	2.6	6
52	Ab initio simulations of Cu binding sites on the N-terminal region of prion protein. <i>Journal of Biological Inorganic Chemistry</i> , 2007, 12, 571-583.	2.6	35
53	Electrostatic interactions with histone tails may bend linker DNA in chromatin. <i>Biopolymers</i> , 2006, 81, 20-28.	2.4	15
54	Modeling H3 histone N-terminal tail and linker DNA interactions. <i>Biopolymers</i> , 2006, 83, 135-147.	2.4	8

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55	Hyaluronan chain conformation and dynamics. Carbohydrate Research, 2005, 340, 959-970.	2.3	39
56	TUNING FORCE-FIELD PARAMETERS BY PRESSURE MEASUREMENTS IN MICRO-CANONICAL SIMULATIONS. International Journal of Modern Physics C, 2004, 15, 205-221.	1.7	1
57	Designing generalized statistical ensembles for numerical simulations of biopolymers. Journal of Chemical Physics, 2004, 121, 10725-10741.	3.0	28
58	Conformational Dynamics of Hyaluronan Oligomers in Solution. 3. Molecular Dynamics from Monte Carlo Replica-Exchange Simulations and Mode-Coupling Diffusion Theory. Macromolecules, 2004, 37, 6197-6209.	4.8	13
59	Modeling the Backbone Dynamics of Reduced and Oxidized Solvated Rat Microsomal Cytochrome b5. Biophysical Journal, 2004, 87, 498-512.	0.5	12
60	Molecular dynamics of C-peptide of ribonuclease A studied by replica-exchange Monte Carlo method and diffusion theory. Chemical Physics Letters, 2003, 380, 609-619.	2.6	18
61	Modeling the dynamics of the solvated SL1 domain of HIV-1 genomic RNA. Biopolymers, 2003, 69, 1-14.	2.4	7
62	A constrained maximum entropy method in polymer statistics. Journal of Chemical Physics, 2003, 119, 8162-8174.	3.0	22
63	Conformational Dynamics of Hyaluronan in Solution. 2. Mode-Coupling Diffusion Approach to Oligomers. Macromolecules, 2002, 35, 286-300.	4.8	12
64	A simple atomistic model for the simulation of the gel phase of lipid bilayers. European Physical Journal E, 2001, 5, 259-274.	1.6	4
65	Modeling the dynamics of a mutated stem-loop in the SL1 domain of HIV-1Lai genomic RNA by 1H-NOESY spectra. Journal of Biomolecular NMR, 2001, 20, 333-349.	2.8	6
66	Polyisoprene local dynamics in solution: Comparison between molecular dynamics simulations and high order diffusion theory. Journal of Chemical Physics, 2001, 114, 1876-1886.	3.0	13
67	Diffusive Dynamics in a Detailed Potential: Application to Biological Macromolecules. Molecular Simulation, 2000, 24, 307-324.	2.0	5
68	Smoluchowski dynamics of the vnd/NK-2 homeodomain from Drosophila melanogaster: Second-order maximum correlation approximation. Biopolymers, 2000, 54, 89-103.	2.4	21
69	Dynamics of a Double Stranded DNA Oligomer: Mode-Coupling Diffusion Approach and Reduced Rigid Fragment Models. Journal of Biomolecular Structure and Dynamics, 2000, 17, 673-685.	3.5	8
70	Molecular dynamics and hybrid Monte Carlo simulations of a sodium bis(2-ethylhexyl)-sulfosuccinate reverse micelle. , 2000, , 20-24.		0
71	Smoluchowski dynamics of the vnd/NK-2 homeodomain from Drosophila melanogaster: Second-order maximum correlation approximation. Biopolymers, 2000, 54, 89-103.	2.4	0
72	Smoluchowski dynamics of the vnd/NK-2 homeodomain from Drosophila melanogaster: First-order mode-coupling approximation. Biopolymers, 1999, 49, 235-254.	2.4	12

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73	Mode-coupling Smoluchowski dynamics of a double-stranded DNA oligomer. , 1999, 50, 613-629.		15
74	Mode-Coupling Smoluchowski Dynamics of Polymers in the Limit of Rigid Structures. Macromolecules, 1999, 32, 506-513.	4.8	22
75	Dynamics of macromolecules and nuclear magnetic relaxation: Application of mode-coupling diffusion theory to DNA, proteins and their complexes. Macromolecular Symposia, 1999, 146, 97-101.	0.7	0
76	The transition state in the isomerization of rhodopsin. Chemical Physics Letters, 1998, 294, 447-453.	2.6	35
77	Parallel computing and molecular dynamics of biological membranes. Nuclear Physics, Section B, Proceedings Supplements, 1998, 63, 985-987.	0.4	1
78	Molecular dynamics with the massively parallel APE computers. Computer Physics Communications, 1997, 106, 53-68.	7.5	5
79	A rigid core-flexible chain model for mesogenic molecules in molecular dynamics simulations of liquid crystals. Journal of Chemical Physics, 1996, 105, 7097-7110.	3.0	30
80	A constrained maximum entropy method for the interpretation of experimental data: Application to the derivation of single particle orientation-conformation distributions from the partially averaged nuclear spin dipolar couplings of n-alkanes dissolved in a liquid crystalline solvent. Journal of Chemical Physics, 1996, 105, 10595-10605.	3.0	15
81	The shape dependence of the solute-solvent interactions in a liquid crystalline phase: A computer simulation study. Journal of Chemical Physics, 1996, 104, 233-241.	3.0	16
82	The enzymatic mechanism of carboxypeptidase: A molecular dynamics study. Proteins: Structure, Function and Bioinformatics, 1994, 18, 186-197.	2.6	24
83	A molecular dynamics study of carboxypeptidase A: effect of protonation of Glu 270. Inorganic Chemistry, 1993, 32, 2207-2211.	4.0	4
84	Molecular dynamics studies on superoxide dismutase and its mutants: the structural and functional role of Arg 143. Journal of the American Chemical Society, 1992, 114, 6994-7001.	13.7	43