Giovanni La Penna

List of Publications by Year
in descending order

83	1,585	331259 21	344852 36
papers	citations	h-index	g-index

88	88	88	1697
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Aggregates Sealed by Ions. Methods in Molecular Biology, 2022, 2340, 309-341.	0.4	3
2	Modelling Protein Plasticity: The Example of Frataxin and Its Variants. Molecules, 2022, 27, 1955.	1.7	2
3	Implementations of replica-permutation and replica sub-permutation methods into LAMMPS. Computer Physics Communications, 2022, 276, 108362.	3.0	2
4	Amyloid Î² Dodecamer Disrupts the Neuronal Membrane More Strongly than the Mature Fibril: Understanding the Role of Oligomers in Neurotoxicity. Journal of Physical Chemistry B, 2022, 126, 3659-3672.	1.2	9
5	Polyphenols as Potential Metal Chelation Compounds Against Alzheimerâ€™s Disease. Journal of Alzheimer's Disease, 2021, 82, S335-S357.	1.2	65
6	Cu(II)â€“Glycerolâ€“N-Ethylmorpholine Complex Stability Revealed by X-ray Spectroscopy. Journal of Physical Chemistry C, 2021, 125, 1483-1492.	1.5	3
7	Probing the Structure of Toxic Amyloid-Î² Oligomers with Electron Spin Resonance and Molecular Modeling. ACS Chemical Neuroscience, 2021, 12, 1150-1161.	1.7	9
8	Measuring Shared Electrons in Extended Molecular Systems: Covalent Bonds from Plane-Wave Representation of Wave Function. Molecules, 2021, 26, 4044.	1.7	1
9	Znâ€Induced Interactions Between SARSâ€CoVâ€2 orf7a and BST2/Tetherin. ChemistryOpen, 2021, 10, 1133-1141.	1.9	11
10	SARS-CoV-2 Virion Stabilization by Zn Binding. Frontiers in Molecular Biosciences, 2020, 7, 222.	1.6	14
11	Emergence of Barrel Motif in Amyloid-Î² Trimer: A Computational Study. Journal of Physical Chemistry B, 2020, 124, 10617-10631.	1.2	12
12	Nanoscopic insights into the surface conformation of neurotoxic amyloid Î² oligomers. RSC Advances, 2020, 10, 21907-21913.	1.7	19
13	Computational Model to Unravel the Function of Amyloid-Î² Peptides in Contact with a Phospholipid Membrane. Journal of Physical Chemistry B, 2020, 124, 3300-3314.	1.2	7
14	Dealing with Cu reduction in X-ray absorption spectroscopy experiments. Metallomics, 2019, 11, 1401-1410.	1.0	11
15	Computational models explain how copper binding to amyloid-Î² peptide oligomers enhances oxidative pathways. Physical Chemistry Chemical Physics, 2019, 21, 8774-8784.	1.3	15
16	When Water Plays an Active Role inÂElectronic Structure. Insights from First-Principles Molecular Dynamics Simulations of Biological Systems. Springer Series on Bio- and Neurosystems, 2019, , 715-753.	0.2	0
17	Towards Highâ€Throughput Modelling of Copper Reactivity Induced by Structural Disorder in Amyloid Peptides. Chemistry - A European Journal, 2018, 24, 5259-5270.	1.7	14
18	Understanding the Exceptional Properties of Nitroacetamides in Water: A Computational Model Including the Solvent. Molecules, 2018, 23, 3308.	1.7	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. Physical Chemistry Chemical Physics, 2018, 20, 24775-24782.	1.3	10
20	Copper Binding Induces Polymorphism in Amyloid-Î² Peptide: Results of Computational Models. Journal of Physical Chemistry B, 2018, 122, 7243-7252.	1.2	17
21	Structural Insights into the Osteopontin-Aptamer Complex by Molecular Dynamics Simulations. Frontiers in Chemistry, 2018, 6, 2.	1.8	16
22	Free Superoxide is an Intermediate in the Production of H₂O₂ by Copper(I)â€Aβ Peptide and O₂. Angewandte Chemie, 2016, 128, 1097-1101.	1.6	18
23	Free Superoxide is an Intermediate in the Production of H₂O₂ by Copper(I)â€Aβ Peptide and O₂. Angewandte Chemie - International Edition, 2016, 55, 1085-1089.	7.2	95
24	Modeling 15N NMR chemical shift changes in protein backbone with pressure. Journal of Chemical Physics, 2016, 145, 085104.	1.2	7
25	Impact of Cu(II) Binding on Structures and Dynamics of Aβ₄₂ Monomer and Dimer: Molecular Dynamics Study. ACS Chemical Neuroscience, 2016, 7, 1348-1363.	1.7	62
26	A first-principle calculation of the XANES spectrum of Cu2+ in water. Journal of Chemical Physics, 2015, 143, 124508.	1.2	24
27	Learning chemistry with multiple first-principles simulations. Molecular Simulation, 2015, 41, 780-787.	0.9	3
28	Dioxygen activation in the Cuâ€“amyloid Î² complex. Physical Chemistry Chemical Physics, 2015, 17, 27270-27274.	1.3	24
29	A Cu-amyloid Î² complex activating Fenton chemistry in Alzheimer's disease: Learning with multiple first-principles simulations. AIP Conference Proceedings, 2014, , .	0.3	4
30	When Water Plays an Active Role in Electronic Structure: Insights from First-Principles Molecular Dynamics Simulations of Biological Systems. Springer Series in Bio-/neuroinformatics, 2014, , 685-710.	0.1	0
31	Metal Ions and Intrinsically Disordered Proteins and Peptides: From Cu/Zn Amyloid-Î² to General Principles. Accounts of Chemical Research, 2014, 47, 2252-2259.	7.6	221
32	Combined EPR and Molecular Modeling Study of PPI Dendrimers Interacting with Copper Ions: Effect of Generation and Maltose Decoration. Journal of Physical Chemistry B, 2014, 118, 12098-12111.	1.2	7
33	Coordination of Metal Ions to Î²-Amyloid Peptide: Impact on Alzheimerâ€™s Disease. Modecular Medicine and Medicinal, 2013, , 127-155.	0.4	0
34	Identifying, By First-Principles Simulations, Cu[Amyloid-Î²] Species Making Fenton-Type Reactions in Alzheimerâ€™s Disease. Journal of Physical Chemistry B, 2013, 117, 16455-16467.	1.2	51
35	Zn induced structural aggregation patterns of Î²-amyloid peptides by first-principle simulations and XAS measurements. Metallomics, 2012, 4, 156-165.	1.0	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. Coordination Chemistry Reviews, 2012, 256, 2234-2244.	9.5	11

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37	Modeling Copper Binding to the Amyloid-Î² Peptide at Different pH: Toward a Molecular Mechanism for Cu Reduction. Journal of Physical Chemistry B, 2012, 116, 11899-11910.	1.2	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. Inorganic Chemistry, 2012, 51, 7897-7902.	1.9	10
39	The mechanism of hydrogen uptake in [NiFe] hydrogenase: first-principles molecular dynamics investigation of a model compound. Journal of Biological Inorganic Chemistry, 2012, 17, 149-164.	1.1	3
40	Exploring the Reactions of Î²-Amyloid (AÎ²) Peptide 1â€“28 with AlIIIand FeIIIIons. Inorganic Chemistry, 2011, 50, 6865-6867.	1.9	42
41	Measuring electron sharing between atoms in first-principle simulations. Theoretical Chemistry Accounts, 2011, 130, 27-36.	0.5	6
42	Wrapped-Around Models for the Lac Operon Complex. Biophysical Journal, 2010, 98, 2964-2973.	0.2	9
43	Modeling the Cu⁺ Binding in the 1â^'16 Region of the Amyloid-Î² Peptide Involved in Alzheimerâ€™s Disease. Journal of Physical Chemistry B, 2010, 114, 15119-15133.	1.2	63
44	Modeling the interplay of glycine protonation and multiple histidine binding of copper in the prion protein octarepeat subdomains. Journal of Biological Inorganic Chemistry, 2009, 14, 361-374.	1.1	27
45	Modeling of the Zn2+ binding in the 1â€“16 region of the amyloid Î² peptide involved in Alzheimerâ€™s disease. Physical Chemistry Chemical Physics, 2009, 11, 6468.	1.3	31
46	Modeling the Free Energy of Polypeptides in Different Environments. Macromolecules, 2008, 41, 2938-2948.	2.2	9
47	Ab Initio Molecular Dynamics of Heme in Cytochrome c. Journal of Physical Chemistry B, 2007, 111, 1157-1164.	1.2	7
48	Anisotropic Internucleosome Interactions and Geometrical Constraints in the Organization of Chromatin. Macromolecules, 2007, 40, 9603-9613.	2.2	7
49	Generalized electrostatic model of the wrapping of DNA around oppositely charged proteins. Biopolymers, 2007, 86, 127-135.	1.2	27
50	Studying the Cu binding sites in the PrP N-terminal region: a test case for ab initio simulations. European Biophysics Journal, 2007, 36, 841-845.	1.2	9
51	Molecular statistics of cytochrome c: structural plasticity and molecular environment. Journal of Biological Inorganic Chemistry, 2007, 12, 180-193.	1.1	6
52	Ab initio simulations of Cu binding sites on the N-terminal region of prion protein. Journal of Biological Inorganic Chemistry, 2007, 12, 571-583.	1.1	35
53	Electrostatic interactions with histone tails may bend linker DNA in chromatin. Biopolymers, 2006, 81, 20-28.	1.2	15
54	Modeling H3 histone N-terminal tail and linker DNA interactions. Biopolymers, 2006, 83, 135-147.	1.2	8

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55	Hyaluronan chain conformation and dynamics. Carbohydrate Research, 2005, 340, 959-970.	1.1	39
56	TUNING FORCE-FIELD PARAMETERS BY PRESSURE MEASUREMENTS IN MICRO-CANONICAL SIMULATIONS. International Journal of Modern Physics C, 2004, 15, 205-221.	0.8	1
57	Designing generalized statistical ensembles for numerical simulations of biopolymers. Journal of Chemical Physics, 2004, 121, 10725-10741.	1.2	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.	2.2	13
59	Modeling the Backbone Dynamics of Reduced and Oxidized Solvated Rat Microsomal Cytochrome b5. Biophysical Journal, 2004, 87, 498-512.	0.2	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.	1.2	18
61	Modeling the dynamics of the solvated SL1 domain of HIV-1 genomic RNA. Biopolymers, 2003, 69, 1-14.	1.2	7
62	A constrained maximum entropy method in polymer statistics. Journal of Chemical Physics, 2003, 119, 8162-8174.	1.2	22
63	Conformational Dynamics of Hyaluronan in Solution. 2. Mode-Coupling Diffusion Approach to Oligomers. Macromolecules, 2002, 35, 286-300.	2.2	12
64	A simple atomistic model for the simulation of the gel phase of lipid bilayers. European Physical Journal E, 2001, 5, 259-274.	0.7	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.	1.6	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.	1.2	13
67	Diffusive Dynamics in a Detailed Potential: Application to Biological Macromolecules. Molecular Simulation, 2000, 24, 307-324.	0.9	5
68	Smoluchowski dynamics of the vnd/NK-2 homeodomain fromDrosophila melanogaster: Second-order maximum correlation approximation. Biopolymers, 2000, 54, 89-103.	1.2	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.	2.0	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 fromDrosophila melanogaster: First-order mode-coupling approximation. Biopolymers, 1999, 49, 235-254.	1.2	12
72	Mode-coupling Smoluchowski dynamics of a double-stranded DNA oligomer. , 1999, 50, 613-629.		15

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73	Mode-Coupling Smoluchowski Dynamics of Polymers in the Limit of Rigid Structures. Macromolecules, 1999, 32, 506-513.	2.2	22
74	Dynamics of macromolecules and nuclear magnetic relaxation: Application of modeâ€coupling diffusion theory to DNA, proteins and their complexes. Macromolecular Symposia, 1999, 146, 97-101.	0.4	0
75	The transition state in the isomerization of rhodopsin. Chemical Physics Letters, 1998, 294, 447-453.	1.2	35
76	Parallel computing and molecular dynamics of biological membranes. Nuclear Physics, Section B, Proceedings Supplements, 1998, 63, 985-987.	0.5	1
77	Molecular dynamics with the massively parallel APE computers. Computer Physics Communications, 1997, 106, 53-68.	3.0	5
78	A rigid coreâ€flexible chain model for mesogenic molecules in molecular dynamics simulations of liquid crystals. Journal of Chemical Physics, 1996, 105, 7097-7110.	1.2	30
79	A constrained maximum entropy method for the interpretation of experimental data: Application to the derivation of single particle orientationâ€conformation distributions from the partially averaged nuclear spin dipolar couplings of nâ€alkanes dissolved in a liquid crystalline solvent. Journal of Chemical Physics, 1996, 105, 10595-10605.	1.2	15
80	The shape dependence of the soluteâ€“solvent interactions in a liquid crystalline phase: A computer simulation study. Journal of Chemical Physics, 1996, 104, 233-241.	1.2	16
81	The enzymatic mechanism of carboxypeptidase: A molecular dynamics study. Proteins: Structure, Function and Bioinformatics, 1994, 18, 186-197.	1.5	24
82	A molecular dynamics study of carboxypeptidase A: effect of protonation of Glu 270. Inorganic Chemistry, 1993, 32, 2207-2211.	1.9	4
83	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.	6.6	43