Alessandro Cembran

List of Publications by Year
in descending order

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56 papers	2,461 citations	218381 26 h-index	233125 45 g-index
57 all docs	57 docs citations	57 times ranked	3137 citing authors

#	Article	IF	Citations
1	On the Mechanism of the cisâ^'trans Isomerization in the Lowest Electronic States of Azobenzene:â€‰ S0, S1, and T1. Journal of the American Chemical Society, 2004, 126, 3234-3243.	6.6	431
2	The Methionine-aromatic Motif Plays a Unique Role in Stabilizing Protein Structure. Journal of Biological Chemistry, 2012, 287, 34979-34991.	1.6	261
3	A theoretical study of the lowest electronic states of azobenzene: the role of torsion coordinate in the cisâ€"trans photoisomerization. Theoretical Chemistry Accounts, 2004, 111, 363-372.	0.5	131
4	Block-Localized Density Functional Theory (BLDFT), Diabatic Coupling, and Their Use in Valence Bond Theory for Representing Reactive Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2009, 5, 2702-2716.	2.3	110
5	From The Cover: The retinal chromophore/chloride ion pair: Structure of the photoisomerization path and interplay of charge transfer and covalent states. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 6255-6260.	3.3	108
6	Structure of the Conical Intersections Driving the cisâ€"trans Photoisomerization of Conjugated MoleculesÂ¶. Photochemistry and Photobiology, 2002, 76, 622.	1.3	91
7	Counterion Controlled Photoisomerization of Retinal Chromophore Models:Â a Computational Investigation. Journal of the American Chemical Society, 2004, 126, 16018-16037.	6.6	89
8	Aborted double bicycle-pedal isomerization with hydrogen bond breaking is the primary event of bacteriorhodopsin proton pumping. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 20172-20177.	3.3	88
9	Structure, Spectroscopy, and Spectral Tuning of the Gas-Phase Retinal Chromophore:â€‰ The Î²-Ionone â€œHandleâ€•and Alkyl Group Effect. Journal of Physical Chemistry A, 2005, 109, 6597-6605.	1.1	83
10	Cyclooctatetraene Computational Photo- and Thermal Chemistry:Â A Reactivity Model for Conjugated Hydrocarbons. Journal of the American Chemical Society, 2002, 124, 13770-13789.	6.6	75
11	Connecting Protein Conformational Dynamics with Catalytic Function As Illustrated in Dihydrofolate Reductase. Biochemistry, 2013, 52, 2036-2049.	1.2	70
12	Complete-active-space self-consistent-field/Amber parameterization of the Lys296?retinal?Glu113 rhodopsin chromophore-counterion system. Theoretical Chemistry Accounts, 2004, 112, 335.	0.5	63
13	Structure of the intersection space associated with Z/E photoisomerization of retinal in rhodopsin proteins. Faraday Discussions, 2004, 127, 179-191.	1.6	60
14	Controlling the Inhibition of the Sarcoplasmic Ca2+-ATPase by Tuning Phospholamban Structural Dynamics. Journal of Biological Chemistry, 2007, 282, 37205-37214.	1.6	55
15	Synchronous Opening and Closing Motions Are Essential for cAMP-Dependent Protein Kinase A Signaling. Structure, 2014, 22, 1735-1743.	1.6	55
16	NMR mapping of protein conformational landscapes using coordinated behavior of chemical shifts upon ligand binding. Physical Chemistry Chemical Physics, 2014, 16, 6508-6518.	1.3	54
17	Oxidation increases the strength of the methionine-aromatic interaction. Nature Chemical Biology, 2016, 12, 860-866.	3.9	53
18	A refinement protocol to determine structure, topology, and depth of insertion of membrane proteins using hybrid solution and solid-state NMR restraints. Journal of Biomolecular NMR, 2009, 44, 195-205.	1.6	48

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19	Dysfunctional conformational dynamics of protein kinase A induced by a lethal mutant of phospholamban hinder phosphorylation. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 3716-3721.	3.3	43
20	Excited-State Singlet Manifold and Oscillatory Features of a Nonatetraeniminium Retinal Chromophore Model. Journal of the American Chemical Society, 2003, 125, 12509-12519.	6.6	41
21	Allostery and Binding Cooperativity of the Catalytic Subunit of Protein Kinase A by NMR Spectroscopy and Molecular Dynamics Simulations. Advances in Protein Chemistry and Structural Biology, 2012, 87, 363-389.	1.0	41
22	On the Function of Pentameric Phospholamban: Ion Channel or Storage Form?. Biophysical Journal, 2009, 96, L60-L62.	0.2	38
23	Tilt and Azimuthal Angles of a Transmembrane Peptide: A Comparison between Molecular Dynamics Calculations and Solid-State NMR Data of Sarcolipin in Lipid Membranes. Biophysical Journal, 2009, 96, 3648-3662.	0.2	33
24	About the intrinsic photochemical properties of the 11-cis retinal chromophore: computational clues for a trap state and a lever effect in Rhodopsin catalysis. Theoretical Chemistry Accounts, 2007, 118, 173-183.	0.5	32
25	Multilevel X-Pol: A Fragment-Based Method with Mixed Quantum Mechanical Representations of Different Fragments. Journal of Physical Chemistry B, 2012, 116, 6781-6788.	1.2	32
26	The Third Dimension of a More Oâ€™Ferrallâ€“Jencks Diagram for Hydrogen Atom Transfer in the Isoelectronic Hydrogen Exchange Reactions of (PhX)₂H^{â€¢} with X = O, NH, and CH₂. Journal of Chemical Theory and Computation, 2012, 8, 4347-4358.	2.3	30
27	On the Interfragment Exchange in the X-Pol Method. Journal of Chemical Theory and Computation, 2010, 6, 2469-2476.	2.3	27
28	Conformational Equilibrium of N-Myristoylated cAMP-Dependent Protein Kinase A by Molecular Dynamics Simulations. Biochemistry, 2012, 51, 10186-10196.	1.2	27
29	Generalized X-Pol Theory and Charge Delocalization States. Journal of Chemical Theory and Computation, 2010, 6, 2402-2410.	2.3	26
30	Role of conformational entropy in the activity and regulation of the catalytic subunit of protein kinase <scp>A</scp>. FEBS Journal, 2013, 280, 5608-5615.	2.2	21
31	A Non-Orthogonal Block-Localized Effective Hamiltonian Approach for Chemical and Enzymatic Reactions. Journal of Chemical Theory and Computation, 2010, 6, 2242-2251.	2.3	18
32	Tuning Sulfur Oxidation States on Thioetherâ€Bridged Peptide Macrocycles for Modulation of Protein Interactions. ChemBioChem, 2017, 18, 1836-1844.	1.3	18
33	Concerted Hydrogen Atom and Electron Transfer Mechanism for Catalysis by Lysine-Specific Demethylase. Journal of Physical Chemistry B, 2013, 117, 8422-8429.	1.2	15
34	Investigating the role of a backbone to substrate hydrogen bond in OMP decarboxylase using a site-specific amide to ester substitution. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 15066-15071.	3.3	15
35	Insight From Animals Resistant to Prion Diseases: Deciphering the Genotype â€“ Morphotype â€“ Phenotype Code for the Prion Protein. Frontiers in Cellular Neuroscience, 2020, 14, 254.	1.8	12
36	FRET Analysis of Ionic Strength Sensors in the Hofmeister Series of Salt Solutions Using Fluorescence Lifetime Measurements. Journal of Physical Chemistry B, 2020, 124, 3447-3458.	1.2	12

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37	Computation of Photochemical Reaction Mechanisms in Organic Chemistry. Theoretical and Computational Chemistry, 2005, 16, 191-223.	0.2	9
38	Flickering dipoles in the gas phase: Structures, internal dynamics, and dipole moments of Î²-naphthol-H2O in its ground and excited electronic states. Journal of Chemical Physics, 2011, 134, 114304.	1.2	9
39	Excited state intramolecular proton transfer in 1-(trifluoroacetylamino)naphthaquinone: a CASPT2//CASSCF computational study. Molecular Physics, 2006, 104, 943-955.	0.8	8
40	Potential energy functions for an intramolecular proton transfer reaction in the ground and excited state. Theoretical Chemistry Accounts, 2007, 118, 211-218.	0.5	8
41	Dynamics of Dystrophinâ€™s Actin-Binding Domain. Biophysical Journal, 2018, 115, 445-454.	0.2	8
42	Kinetic Isotope Effects from Hybrid Classical and Quantum Path Integral Computations. RSC Biomolecular Sciences, 2009, , 105-131.	0.4	5
43	Internal Dynamics of an Analytically Coarse-Grained Protein. Journal of Chemical Theory and Computation, 2010, 6, 3601-3612.	2.3	4
44	Mechanical Unfolding of Spectrin Repeats Induces Water-Molecule Ordering. Biophysical Journal, 2020, 118, 1076-1089.	0.2	3
45	Retinal chromophore photoinduced molecular motion and reactivity: isolated conditions and counterion effects. Journal of Computational Methods in Sciences and Engineering, 2002, 2, 431-439.	0.1	0
46	Structure of the Conical Intersections Driving the cisâ€”trans Photoisomerization of Conjugated Molecules. ChemInform, 2003, 34, no.	0.1	0
47	Solid-State NMR Structures of Phospholamban or Sarcolipin Bound to Calcium ATPase (SERCA) Reveal the Mode of Inhibition. Biophysical Journal, 2014, 106, 585a.	0.2	0
48	Quantitative Interpretation of Chemical Shifts Enables Mapping Proteins Conformational Landscape. Biophysical Journal, 2014, 106, 807a.	0.2	0
49	Sarcolipin-Mediated Regulation of SERCA by Computer Simulations. Biophysical Journal, 2015, 108, 384a.	0.2	0
50	Dysfunctional Conformational Dynamics of Protein Kinase a from R14 Deletion of Phospholamban. Biophysical Journal, 2015, 108, 529a.	0.2	0
51	Oxidation Increases the Strength of the Methionine-Aromatic Interaction. Biophysical Journal, 2015, 108, 17a.	0.2	0
52	Spectroscopic and Computational Analysis of Dystrophin Regulation of Actin Dynamics. Biophysical Journal, 2016, 110, 128a.	0.2	0
53	Molecular Dynamics Simulation and Markov State Model Reveal Irregular Metastable Conformation and Allostery In DNAJB-PKAc. Biophysical Journal, 2016, 110, 51a-52a.	0.2	0
54	Hydrophobic Interactions Elicit Cooperative Response in Dystrophin. Biophysical Journal, 2016, 110, 362a.	0.2	0

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55	Atomic-Level Characterization of the Structural Dynamics of Azurin Variants with Tuned Reduction Potentials. Biophysical Journal, 2018, 114, 521a.	0.2	0
56	The Role of Hydrophobic Interactions and Water Dynamics Around Dystrophin Spectrin Repeats. Biophysical Journal, 2018, 114, 525a.	0.2	0