Laura Zanetti-Polzi

List of Publications by Year
in descending order

43	848	430754	501076
papers	citations	18 h-index	28 g-index

48	48	48	1052
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A general statistical mechanical model for fluid system thermodynamics: Application to sub- and super-critical water. Journal of Chemical Physics, 2022, 156, 044506.	1.2	3
2	Low- and high-density forms of liquid water revealed by a new medium-range order descriptor. Journal of Molecular Liquids, 2022, 355, 118922.	2.3	11
3	Photophysical and Computational Insights into Ag(I) Complexation of Porphyrinic Covalent Cages Equipped with Triazoles-Incorporating Linkers. Journal of Physical Chemistry B, 2022, 126, 3450-3459.	1.2	0
4	Evidence for a high pK_a of an aspartic acid residue in the active site of CALB by a fully atomistic multiscale approach. Journal of Biomolecular Structure and Dynamics, 2022, , 1-8.	2.0	2
5	A computational insight into the relationship between side chain IR line shapes and local environment in fibril-like structures. Journal of Chemical Physics, 2021, 154, 084105.	1.2	1
6	Tuning Proton Transfer Thermodynamics in SARS-CoV-2 Main Protease: Implications for Catalysis and Inhibitor Design. Journal of Physical Chemistry Letters, 2021, 12, 4195-4202.	2.1	19
7	Segregation on the nanoscale coupled to liquid water polyamorphism in supercooled aqueous ionic-liquid solution. Journal of Chemical Physics, 2021, 155, 104502.	1.2	3
8	Inhibitor binding influences the protonation states of histidines in SARS-CoV-2 main protease. Chemical Science, 2021, 12, 1513-1527.	3.7	47
9	Allosteric Control of Naphthalene Diimide Encapsulation and Electron Transfer in Porphyrin Containers: Photophysical Studies and Molecular Dynamics Simulation. Chemistry - A European Journal, 2020, 26, 17514-17524.	1.7	7
10	Supercomputer-Based Ensemble Docking Drug Discovery Pipeline with Application to Covid-19. Journal of Chemical Information and Modeling, 2020, 60, 5832-5852.	2.5	134
11	Fully Atomistic Multiscale Approach for pK_a Prediction. Journal of Physical Chemistry B, 2020, 124, 4712-4722.	1.2	10
12	Modeling amino-acid side chain infrared spectra: the case of carboxylic residues. Physical Chemistry Chemical Physics, 2020, 22, 3008-3016.	1.3	10
13	The Interaction between Amyloid Prefibrillar Oligomers of Salmon Calcitonin and a Lipid-Raft Model: Molecular Mechanisms Leading to Membrane Damage, Ca2+-Influx and Neurotoxicity. Biomolecules, 2020, 10, 58.	1.8	3
14	Cooperative proteinâ€“solvent tuning of proton transfer energetics: carbonic anhydrase as a case study. Physical Chemistry Chemical Physics, 2020, 22, 19975-19981.	1.3	3
15	Hydration Shell of Antifreeze Proteins: Unveiling the Role of Non-Ice-Binding Surfaces. Journal of Physical Chemistry B, 2019, 123, 6474-6480.	1.2	20
16	Interpretation of Experimental Soret Bands of Porphyrins in Flexible Covalent Cages and in Their Related Ag(I) Fixed Complexes. Journal of Physical Chemistry C, 2019, 123, 13094-13103.	1.5	17
17	Evidence of a Thermodynamic Ramp for Hole Hopping to Protect a Redox Enzyme from Oxidative Damage. Journal of Physical Chemistry Letters, 2019, 10, 1450-1456.	2.1	10
18	Tip-Enhanced Infrared Difference-Nanospectroscopy of the Proton Pump Activity of Bacteriorhodopsin in Single Purple Membrane Patches. Nano Letters, 2019, 19, 3104-3114.	4.5	36

#	Article	IF	Citations
19	Difference mid-IR nanospectroscopy on individual patches of purple membranes: the proton pump activity of bacteriorhodopsin at the nanoscale. , 2019, , .		0
20	On the nature of solvatochromic effect: The riboflavin absorption spectrum as a case study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 192, 451-457.	2.0	8
21	A quantitative connection of experimental and simulated folding landscapes by vibrational spectroscopy. Chemical Science, 2018, 9, 9002-9011.	3.7	20
22	Extending the perturbed matrix method beyond the dipolar approximation: comparison of different levels of theory. Physical Chemistry Chemical Physics, 2018, 20, 24369-24378.	1.3	49
23	Tyrosine absorption spectroscopy: Backbone protonation effects on the side chain electronic properties. Journal of Computational Chemistry, 2018, 39, 1747-1756.	1.5	17
24	Theoretical modeling of the absorption spectrum of aqueous riboflavin. Chemical Physics Letters, 2017, 669, 119-124.	1.2	37
25	Computational evidence support the hypothesis of neuroglobin also acting as an electron transfer species. Journal of Biological Inorganic Chemistry, 2017, 22, 615-623.	1.1	24
26	Computational investigation of the electron transfer complex between neuroglobin and cytochrome c. Supramolecular Chemistry, 2017, 29, 846-852.	1.5	2
27	Parallel folding pathways of Fip35 WW domain explained by infrared spectra and their computer simulation. FEBS Letters, 2017, 591, 3265-3275.	1.3	12
28	Alternative Electron-Transfer Channels Ensure Ultrafast Deactivation of Light-Induced Excited States in Riboflavin Binding Protein. Journal of Physical Chemistry Letters, 2017, 8, 3321-3327.	2.1	21
29	Theoretical-computational characterization of the temperature-dependent folding thermodynamics of aÎ²-hairpin peptide. Chemical Physics Letters, 2016, 659, 247-251.	1.2	1
30	Extending the essential dynamics analysis to investigate molecular properties: application to the redox potential of proteins. Physical Chemistry Chemical Physics, 2016, 18, 18450-18459.	1.3	18
31	A dynamical approach to non-adiabatic electron transfers at the bio-inorganic interface. Physical Chemistry Chemical Physics, 2016, 18, 10538-10549.	1.3	11
32	A few key residues determine the high redox potential shift in azurin mutants. Organic and Biomolecular Chemistry, 2015, 13, 11003-11013.	1.5	35
33	Surface Packing Determines the Redox Potential Shift of Cytochrome c Adsorbed on Gold. Journal of the American Chemical Society, 2014, 136, 12929-12937.	6.6	39
34	Simulation of the Amide I Infrared Spectrum in Photoinduced Peptide Folding/Unfolding Transitions. Journal of Physical Chemistry B, 2013, 117, 12383-12390.	1.2	17
35	Modeling triplet flavin-indole electron transfer and interradical dipolar interaction: a perturbative approach. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	14
36	A Theoretical Reappraisal of Polylysine in the Investigation of Secondary Structure Sensitivity of Infrared Spectra. Journal of Physical Chemistry B, 2012, 116, 3353-3360.	1.2	19

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37	New Insight into the IR-Spectra/Structure Relationship in Amyloid Fibrils: A Theoretical Study on a Prion Peptide. Journal of the American Chemical Society, 2011, 133, 11414-11417.	6.6	28
38	Analysis of Infrared Spectra of Î²-Hairpin Peptides As Derived from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2011, 115, 11872-11878.	1.2	11
39	Structure of the lipodepsipeptide syringomycin E in phospholipids and sodium dodecylsulphate micelle studied by circular dichroism, NMR spectroscopy and molecular dynamics. Biochimica Et Biophysica Acta - Biomembranes, 2011, 1808, 2102-2110.	1.4	15
40	Modeling quantum vibrational excitations in condensed-phase molecular systems. Theoretical Chemistry Accounts, 2011, 129, 31-43.	0.5	26
41	On the origin of IR spectral changes upon protein folding. Chemical Physics Letters, 2010, 488, 213-218.	1.2	30
42	Structural, thermodynamic, and kinetic properties of Gramicidin analogue GS6 studied by molecular dynamics simulations and statistical mechanics. Biopolymers, 2009, 91, 1154-1160.	1.2	1
43	Calcitonin Forms Oligomeric Pore-Like Structures in Lipid Membranes. Biophysical Journal, 2006, 91, 2275-2281.	0.2	52