Laura Zanetti-Polzi

List of Publications by Year
in descending order

43	848	430442	500791
papers	citations	18 h-index	28 g-index

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

#	Article	IF	Citations
1	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
2	Calcitonin Forms Oligomeric Pore-Like Structures in Lipid Membranes. Biophysical Journal, 2006, 91, 2275-2281.	0.2	52
3	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
4	Inhibitor binding influences the protonation states of histidines in SARS-CoV-2 main protease. Chemical Science, 2021, 12, 1513-1527.	3.7	47
5	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
6	Theoretical modeling of the absorption spectrum of aqueous riboflavin. Chemical Physics Letters, 2017, 669, 119-124.	1.2	37
7	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
8	A few key residues determine the high redox potential shift in azurin mutants. Organic and Biomolecular Chemistry, 2015, 13, 11003-11013.	1.5	35
9	On the origin of IR spectral changes upon protein folding. Chemical Physics Letters, 2010, 488, 213-218.	1.2	30
10	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
11	Modeling quantum vibrational excitations in condensed-phase molecular systems. Theoretical Chemistry Accounts, 2011, 129, 31-43.	0.5	26
12	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
13	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
14	A quantitative connection of experimental and simulated folding landscapes by vibrational spectroscopy. Chemical Science, 2018, 9, 9002-9011.	3.7	20
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	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
17	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
18	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

#	Article	IF	Citations
19	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
20	Tyrosine absorption spectroscopy: Backbone protonation effects on the side chain electronic properties. Journal of Computational Chemistry, 2018, 39, 1747-1756.	1.5	17
21	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
22	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
23	Modeling triplet flavin-indole electron transfer and interradical dipolar interaction: a perturbative approach. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	14
24	Parallel folding pathways of Fip35 WW domain explained by infrared spectra and their computer simulation. FEBS Letters, 2017, 591, 3265-3275.	1.3	12
25	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
26	A dynamical approach to non-adiabatic electron transfers at the bio-inorganic interface. Physical Chemistry Chemical Physics, 2016, 18, 10538-10549.	1.3	11
27	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
28	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
29	Fully Atomistic Multiscale Approach for pK_a Prediction. Journal of Physical Chemistry B, 2020, 124, 4712-4722.	1.2	10
30	Modeling amino-acid side chain infrared spectra: the case of carboxylic residues. Physical Chemistry Chemical Physics, 2020, 22, 3008-3016.	1.3	10
31	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
32	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
33	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
34	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
35	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
36	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

#	Article	IF	Citations
37	Computational investigation of the electron transfer complex between neuroglobin and cytochrome c. Supramolecular Chemistry, 2017, 29, 846-852.	1.5	2
38	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
39	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
40	Theoretical-computational characterization of the temperature-dependent folding thermodynamics of aÎ²-hairpin peptide. Chemical Physics Letters, 2016, 659, 247-251.	1.2	1
41	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
42	Difference mid-IR nanospectroscopy on individual patches of purple membranes: the proton pump activity of bacteriorhodopsin at the nanoscale. , 2019, , .		0
43	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