Isabella Daidone

List of Publications by Year
in descending order

85 papers	2,208 citations	230014 27 h-index	299063 42 g-index
87 all docs	87 docs citations	87 times ranked	2743 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	Hit Expansion of a Noncovalent SARS-CoV-2 Main Protease Inhibitor. ACS Pharmacology and Translational Science, 2022, 5, 255-265.	2.5	17
3	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
4	High density water clusters observed at high concentrations of the macromolecular crowder PEG400. Journal of Molecular Liquids, 2022, 357, 119038.	2.3	2
5	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
6	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
7	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
8	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
9	High Water Density at Non-Ice-Binding Surfaces Contributes to the Hyperactivity of Antifreeze Proteins. Journal of Physical Chemistry Letters, 2021, 12, 8777-8783.	2.1	11
10	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
11	Inhibitor binding influences the protonation states of histidines in SARS-CoV-2 main protease. Chemical Science, 2021, 12, 1513-1527.	3.7	47
12	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
13	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
14	Fully Atomistic Multiscale Approach for pK_a Prediction. Journal of Physical Chemistry B, 2020, 124, 4712-4722.	1.2	10
15	Length-scale dependence of protein hydration-shell density. Physical Chemistry Chemical Physics, 2020, 22, 7340-7347.	1.3	5
16	Modeling amino-acid side chain infrared spectra: the case of carboxylic residues. Physical Chemistry Chemical Physics, 2020, 22, 3008-3016.	1.3	10
17	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
18	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

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19	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
20	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
21	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
22	Difference mid-IR nanospectroscopy on individual patches of purple membranes: the proton pump activity of bacteriorhodopsin at the nanoscale. , 2019, , .		0
23	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
24	A quantitative connection of experimental and simulated folding landscapes by vibrational spectroscopy. Chemical Science, 2018, 9, 9002-9011.	3.7	20
25	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
26	Tyrosine absorption spectroscopy: Backbone protonation effects on the side chain electronic properties. Journal of Computational Chemistry, 2018, 39, 1747-1756.	1.5	17
27	Theoretical modeling of the absorption spectrum of aqueous riboflavin. Chemical Physics Letters, 2017, 669, 119-124.	1.2	37
28	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
29	Computational investigation of the electron transfer complex between neuroglobin and cytochrome c. Supramolecular Chemistry, 2017, 29, 846-852.	1.5	2
30	Parallel folding pathways of Fip35 WW domain explained by infrared spectra and their computer simulation. FEBS Letters, 2017, 591, 3265-3275.	1.3	12
31	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
32	Photoexcitation and relaxation kinetics of molecular systems in solution: towards a complete in silico model. Physical Chemistry Chemical Physics, 2016, 18, 28919-28931.	1.3	19
33	Conformational Change in the Mechanism of Inclusion of Ketoprofen in Î²-Cyclodextrin: NMR Spectroscopy, Ab Initio Calculations, Molecular Dynamics Simulations, and Photoreactivity. Journal of Physical Chemistry B, 2016, 120, 10668-10678.	1.2	15
34	Theoretical-computational characterization of the temperature-dependent folding thermodynamics of aÎ²-hairpin peptide. Chemical Physics Letters, 2016, 659, 247-251.	1.2	1
35	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
36	Î²-Structure within the Denatured State of the Helical Protein Domain BBL. Journal of Molecular Biology, 2015, 427, 3166-3176.	2.0	6

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37	Monitoring the Folding Kinetics of a Î²-Hairpin by Time-Resolved IR Spectroscopy in Silico. Journal of Physical Chemistry B, 2015, 119, 4849-4856.	1.2	11
38	A few key residues determine the high redox potential shift in azurin mutants. Organic and Biomolecular Chemistry, 2015, 13, 11003-11013.	1.5	35
39	How the Reorganization Free Energy Affects the Reduction Potential of Structurally Homologous Cytochromes. Journal of Physical Chemistry Letters, 2014, 5, 1534-1540.	2.1	19
40	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
41	Theoretical-computational modeling of photo-induced charge separation spectra and charge recombination kinetics in solution. Physical Chemistry Chemical Physics, 2014, 16, 20624-20638.	1.3	15
42	Unambiguous Assignment of Reduction Potentials in Diheme Cytochromes. Journal of Physical Chemistry B, 2014, 118, 7554-7560.	1.2	20
43	Structure and solvation properties of aqueous sulfobetaine micelles in the presence of organic spin probes: a Molecular Dynamics simulation study. Structural Chemistry, 2013, 24, 945-953.	1.0	9
44	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
45	Toward a Realistic Modeling of the Photophysics of Molecular Building Blocks for Energy Harvesting: The Charge-Transfer State in 4,7-Dithien-2-yl-2,1,3-benzothiadiazole As a Case Study. Journal of Physical Chemistry C, 2013, 117, 13785-13797.	1.5	13
46	Modeling triplet flavin-indole electron transfer and interradical dipolar interaction: a perturbative approach. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	14
47	A general statistical mechanical approach for modeling redox thermodynamics: the reaction and reorganization free energies. RSC Advances, 2013, 3, 19657.	1.7	16
48	Structural and dynamical properties of KTSâ€disintegrins: A comparison between Obtustatin and Lebestatin. Biopolymers, 2013, 99, 47-54.	1.2	12
49	On the structural affinity of macromolecules with different biological properties: Molecular dynamics simulations of a series of TEM-1 mutants. Biochemical and Biophysical Research Communications, 2013, 436, 666-671.	1.0	3
50	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
51	A general theoretical model for electron transfer reactions in complex systems. Physical Chemistry Chemical Physics, 2012, 14, 1360-1370.	1.3	35
52	Alteration of Water Structure by Peptide Clusters Revealed by Neutron Scattering in the Small-Angle Region (below 1ÂÃ…â^'1). Biophysical Journal, 2012, 103, 1518-1524.	0.2	5
53	Essential dynamics: foundation and applications. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 762-770.	6.2	99
54	The Reversible Opening of Water Channels in Cytochrome c Modulates the Heme Iron Reduction Potential. Journal of the American Chemical Society, 2012, 134, 13670-13678.	6.6	71

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55	Configurational subdiffusion of peptides: A network study. Physical Review E, 2011, 83, 021902.	0.8	12
56	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
57	Molecular Origin of Gerstmann-StrÃussler-Scheinker Syndrome: Insight from Computer Simulation of an Amyloidogenic Prion Peptide. Biophysical Journal, 2011, 100, 3000-3007.	0.2	11
58	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
59	Conformational study of bovine lactoferricin in membrane-micking conditions by molecular dynamics simulation and circular dichroism. BioMetals, 2011, 24, 259-268.	1.8	10
60	Modeling quantum vibrational excitations in condensed-phase molecular systems. Theoretical Chemistry Accounts, 2011, 129, 31-43.	0.5	26
61	Dynamical fingerprints for probing individual relaxation processes in biomolecular dynamics with simulations and kinetic experiments. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 4822-4827.	3.3	105
62	Structured Pathway across the Transition State for Peptide Folding Revealed by Molecular Dynamics Simulations. PLoS Computational Biology, 2011, 7, e1002137.	1.5	7
63	Theoretical-computational modelling of infrared spectra in peptides and proteins: a new frontier for combined theoretical-experimental investigations. Current Opinion in Structural Biology, 2010, 20, 155-161.	2.6	35
64	On the origin of IR spectral changes upon protein folding. Chemical Physics Letters, 2010, 488, 213-218.	1.2	30
65	Hydrogen-Bond Driven Loop-Closure Kinetics in Unfolded Polypeptide Chains. PLoS Computational Biology, 2010, 6, e1000645.	1.5	44
66	Mechanism of DNA Recognition by the Restriction Enzyme EcoRV. Journal of Molecular Biology, 2010, 401, 415-432.	2.0	24
67	Common Folding Mechanism of a Î²-Hairpin Peptide via Non-native Turn Formation Revealed by Unbiased Molecular Dynamics Simulations. Journal of the American Chemical Society, 2009, 131, 18147-18152.	6.6	36
68	Instantaneous Normal Modes and the Protein Glass Transition. Biophysical Journal, 2009, 96, 476-484.	0.2	12
69	Chargeâ€Based Interactions between Peptides Observed as the Dominant Force for Association in Aqueous Solution. Angewandte Chemie - International Edition, 2008, 47, 9059-9062.	7.2	39
70	Subdiffusion in Peptides Originates from the Fractal-Like Structure of Configuration Space. Physical Review Letters, 2008, 100, 188103.	2.9	63
71	Solvent Electrostriction-Driven Peptide Folding Revealed by Quasi-Gaussian Entropy Theory and Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2008, 112, 11155-11163.	1.2	9
72	Protein Folding Pathways Revealed by Essential Dynamics Sampling. Journal of Chemical Theory and Computation, 2008, 4, 1940-1948.	2.3	13

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73	Dehydration-driven solvent exposure of hydrophobic surfaces as a driving force in peptide folding. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 15230-15235.	3.3	72
74	Statistical mechanical modelling of chemical reactions in complex systems: the kinetics of the Haem carbon monoxide bindingâ€“unbinding reaction in Myoglobin. Theoretical Chemistry Accounts, 2007, 117, 637-647.	0.5	28
75	Theoretical modeling of chemical reactions in complex environments: the intramolecular proton transfer in aqueous malonaldehyde. Journal of Physical Organic Chemistry, 2006, 19, 518-530.	0.9	28
76	Aggregation of small peptides studied by molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2006, 65, 914-921.	1.5	19
77	Molecular dynamics simulation of the aggregation of the core-recognition motif of the islet amyloid polypeptide in explicit water. Proteins: Structure, Function and Bioinformatics, 2005, 59, 519-527.	1.5	49
78	Thermodynamic and kinetic characterization of a Î²-hairpin peptide in solution: An extended phase space sampling by molecular dynamics simulations in explicit water. Proteins: Structure, Function and Bioinformatics, 2005, 59, 510-518.	1.5	49
79	Theoretical Characterization of Î±-Helix and Î²-Hairpin Folding Kinetics. Journal of the American Chemical Society, 2005, 127, 14825-14832.	6.6	43
80	Molecular Dynamics Simulation of Sperm Whale Myoglobin: Effects of Mutations and Trapped CO on the Structure and Dynamics of Cavities. Biophysical Journal, 2005, 89, 465-474.	0.2	93
81	Î²-Hairpin conformation of fibrillogenic peptides: Structure and Î±-Î² transition mechanism revealed by molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2004, 57, 198-204.	1.5	85
82	A molecular dynamics study of acylphosphatase in aggregation-promoting conditions: The influence of trifluoroethanol/water solvent. Biopolymers, 2004, 75, 491-496.	1.2	4
83	Investigating the Accessibility of the Closed Domain Conformation of Citrate Synthase using Essential Dynamics Sampling. Journal of Molecular Biology, 2004, 339, 515-525.	2.0	35
84	Molecular Dynamics Simulation of Protein Folding by Essential Dynamics Sampling: Folding Landscape of Horse Heart Cytochrome c. Biophysical Journal, 2003, 85, 2865-2871.	0.2	67
85	Selective Excitation of Native Fluctuations during Thermal Unfolding Simulations: Horse Heart Cytochrome c as a Case Study. Biophysical Journal, 2003, 84, 1876-1883.	0.2	45