Andrea Amadei

List of Publications by Year
in descending order

133 papers	6,121 citations	147566 31 h-index	76769 74 g-index
135 all docs	135 docs citations	135 times ranked	5499 citing authors

#	Article	IF	Citations
1	Essential dynamics of proteins. Proteins: Structure, Function and Bioinformatics, 1993, 17, 412-425.	1.5	2,927
2	On the convergence of the conformational coordinates basis set obtained by the essential dynamics analysis of proteins' molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 1999, 36, 419-424.	1.5	277
3	Extended Molecular Dynamics Simulation of the Carbon Monoxide Migration in Sperm Whale Myoglobin. Biophysical Journal, 2004, 86, 3855-3862.	0.2	129
4	A molecular dynamics study of the 41â€56 Î²â€hairpin from B1 domain of protein G. Protein Science, 1999, 8, 2130-2143.	3.1	109
5	Essential dynamics: foundation and applications. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 762-770.	6.2	99
6	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
7	Effect of High Exogenous Electric Pulses on Protein Conformation: Myoglobin as a Case Study. Journal of Physical Chemistry B, 2013, 117, 2273-2279.	1.2	85
8	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
9	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
10	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
11	Theoretical characterization of electronic states in interacting chemical systems. Journal of Chemical Physics, 2009, 130, 084109.	1.2	66
12	In vitropreferential topoisomerization of bent DNA. Nucleic Acids Research, 1989, 17, 8463-8474.	6.5	63
13	Extension of the perturbed matrix method: application to a water molecule. Chemical Physics Letters, 2002, 365, 450-456.	1.2	51
14	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
15	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
16	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
17	A mean field approach for molecular simulations of fluid systems. Journal of Chemical Physics, 2005, 122, 154109.	1.2	46
18	Mechanics and dynamics of B1 domain of protein G: Role of packing and surface hydrophobic residues. Protein Science, 1999, 8, 147-160.	3.1	46

#	Article	IF	Citations
19	On the Nature of DNA Hyperchromic Effect. Journal of Physical Chemistry B, 2013, 117, 8697-8704.	1.2	44
20	Theoretical Characterization of Î±-Helix and Î²-Hairpin Folding Kinetics. Journal of the American Chemical Society, 2005, 127, 14825-14832.	6.6	43
21	Theoretical modeling of UV-Vis absorption and emission spectra in liquid state systems including vibrational and conformational effects: Explicit treatment of the vibronic transitions. Journal of Chemical Physics, 2014, 140, 164104.	1.2	42
22	Identification of functional and unfolding motions of cutinase as obtained from molecular dynamics computer simulations. , 1998, 33, 253-264.		40
23	Theoretical modeling of the valence UV spectra of 1,2,3-triazine and uracil in solution. Physical Chemistry Chemical Physics, 2006, 8, 1385.	1.3	39
24	Theoretical modeling of the absorption spectrum of aqueous riboflavin. Chemical Physics Letters, 2017, 669, 119-124.	1.2	37
25	The Effect of Protein Conformational Flexibility on the Electronic Properties of a Chromophore. Biophysical Journal, 2003, 84, 2805-2813.	0.2	36
26	Mixed Quantum-Classical Methods for Molecular Simulations of Biochemical Reactions With Microwave Fields: The Case Study of Myoglobin. IEEE Transactions on Microwave Theory and Techniques, 2008, 56, 2511-2519.	2.9	36
27	Theoretical modeling of UV-Vis absorption and emission spectra in liquid state systems including vibrational and conformational effects: The vertical transition approximation. Journal of Chemical Physics, 2013, 139, 114102.	1.2	36
28	Conformational fluctuations and electronic properties in myoglobin. Journal of Computational Chemistry, 2004, 25, 974-984.	1.5	35
29	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
30	A general theoretical model for electron transfer reactions in complex systems. Physical Chemistry Chemical Physics, 2012, 14, 1360-1370.	1.3	35
31	A few key residues determine the high redox potential shift in azurin mutants. Organic and Biomolecular Chemistry, 2015, 13, 11003-11013.	1.5	35
32	In silico characterization of protein partial molecular volumes and hydration shells. Physical Chemistry Chemical Physics, 2015, 17, 31270-31277.	1.3	35
33	Theoretical modeling of vibroelectronic quantum states in complex molecular systems: Solvated carbon monoxide, a test case. Journal of Chemical Physics, 2005, 122, 124506.	1.2	34
34	Theoretical Modeling of Enzyme Reaction Chemistry:Â The Electron Transfer of the Reduction Mechanism in CuZn Superoxide Dismutase. Journal of Physical Chemistry B, 2004, 108, 16255-16260.	1.2	31
35	Theoretical Characterisation of the Electronic Excitation in Liquid Water. ChemPhysChem, 2005, 6, 53-58.	1.0	31
36	The Kinetics of Ligand Migration in Crystallized Myoglobin as Revealed by Molecular Dynamics Simulations. Biophysical Journal, 2008, 94, 4277-4281.	0.2	31

#	Article	IF	Citations
37	On the origin of IR spectral changes upon protein folding. Chemical Physics Letters, 2010, 488, 213-218.	1.2	30
38	The conformation of constitutive DNA interaction sites for eukaryotic DNA topoisomerase I on intrinsically curved DNAs. Biochimica Et Biophysica Acta Gene Regulatory Mechanisms, 1991, 1129, 73-82.	2.4	28
39	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
40	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
41	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
42	Modeling quantum vibrational excitations in condensed-phase molecular systems. Theoretical Chemistry Accounts, 2011, 129, 31-43.	0.5	26
43	Theoretical Modeling of Enzyme Reactions:â€‰ The Thermodynamics of Formation of Compound 0 in Horseradish Peroxidase. Journal of Physical Chemistry B, 2008, 112, 3184-3192.	1.2	24
44	Theoretical Characterization of Carbon Monoxide Vibrational Spectrum in Sperm Whale Myoglobin Distal Pocket. Biophysical Journal, 2007, 92, 3442-3447.	0.2	23
45	Modeling of Chemical Reactions in Micelle: Water-Mediated Ketoâ€“Enol Interconversion As a Case Study. Journal of Physical Chemistry B, 2011, 115, 8102-8111.	1.2	23
46	Theoretical characterization of temperature and density dependence of liquid water electronic excitation energy: Comparison with recent experimental data. Journal of Chemical Physics, 2008, 128, 021103.	1.2	22
47	A DFT Study of the Low-Lying Singlet Excited States of the All-Trans Peridinin in vacuo. Journal of Physical Chemistry A, 2004, 108, 6763-6770.	1.1	21
48	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
49	Unambiguous Assignment of Reduction Potentials in Diheme Cytochromes. Journal of Physical Chemistry B, 2014, 118, 7554-7560.	1.2	20
50	A quantitative connection of experimental and simulated folding landscapes by vibrational spectroscopy. Chemical Science, 2018, 9, 9002-9011.	3.7	20
51	Aggregation of small peptides studied by molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2006, 65, 914-921.	1.5	19
52	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
53	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
54	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

#	Article	IF	Citations
55	Statistical Mechanics and Thermodynamics of Simulated Ionic Solutions. Journal of Physical Chemistry B, 2002, 106, 11843-11848.	1.2	18
56	Theoretical modeling of the spectroscopic absorption properties of luciferin and oxyluciferin: A critical comparison with recent experimental studies. Chemical Physics, 2012, 392, 205-214.	0.9	18
57	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
58	Kinetics of Carbon Monoxide Migration and Binding in Solvated Myoglobin as Revealed by Molecular Dynamics Simulations and Quantum Mechanical Calculations. Journal of Physical Chemistry B, 2009, 113, 16346-16353.	1.2	17
59	Characterization of Electronic Properties in Complex Molecular Systems: Modeling of a Micropolarity Probe. Journal of Physical Chemistry B, 2010, 114, 1915-1924.	1.2	17
60	Kinetics of Carbon Monoxide Migration and Binding in Solvated Neuroglobin As Revealed by Molecular Dynamics Simulations and Quantum Mechanical Calculations. Journal of Physical Chemistry B, 2011, 115, 2436-2446.	1.2	17
61	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
62	Tyrosine absorption spectroscopy: Backbone protonation effects on the side chain electronic properties. Journal of Computational Chemistry, 2018, 39, 1747-1756.	1.5	17
63	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
64	On the Effect of a Point Mutation on the Reactivity of CuZn Superoxide Dismutase:Â A Theoretical Study. Journal of Physical Chemistry B, 2006, 110, 7538-7544.	1.2	16
65	A general statistical mechanical approach for modeling redox thermodynamics: the reaction and reorganization free energies. RSC Advances, 2013, 3, 19657.	1.7	16
66	Essential dynamics for the study of microstructures in liquids. Journal of Computational Chemistry, 2015, 36, 399-407.	1.5	16
67	The self-association equilibria of doxorubicin at high concentration and ionic strength characterized by fluorescence spectroscopy and molecular dynamics simulations. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2019, 577, 517-522.	2.3	16
68	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
69	The unfolding effects on the protein hydration shell and partial molar volume: a computational study. Physical Chemistry Chemical Physics, 2016, 18, 28175-28182.	1.3	15
70	Flexible and Comprehensive Implementation of MD-PMM Approach in a General and Robust Code. Journal of Chemical Theory and Computation, 2017, 13, 5506-5514.	2.3	15
71	Can a synthetic thread act as an electrochemically switchable molecular device?. Chemical Communications, 2008, , 3399.	2.2	14
72	Modeling triplet flavin-indole electron transfer and interradical dipolar interaction: a perturbative approach. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	14

#	Article	IF	Citations
73	Photoinduced electron transfer in a dichromophoric peptide: a numerical experiment. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	14
74	Protein Folding Pathways Revealed by Essential Dynamics Sampling. Journal of Chemical Theory and Computation, 2008, 4, 1940-1948.	2.3	13
75	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
76	Molecular mechanisms of activation in CDK2. Journal of Biomolecular Structure and Dynamics, 2014, 32, 1929-1935.	2.0	13
77	Theoretical Characterization of the Reduction Potentials of Nucleic Acids in Solution. Journal of Chemical Theory and Computation, 2021, 17, 1301-1307.	2.3	13
78	Theoretical study of intramolecular charge transfer in Ï€-conjugated oligomers. Chemical Physics Letters, 2007, 434, 194-199.	1.2	12
79	Theoretical calculation of the pyrene emission properties in different solvents. Chemical Physics Letters, 2015, 639, 17-22.	1.2	12
80	Parallel folding pathways of Fip35 WW domain explained by infrared spectra and their computer simulation. FEBS Letters, 2017, 591, 3265-3275.	1.3	12
81	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
82	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
83	Density discriminates between thermophilic and mesophilic proteins. Journal of Biomolecular Structure and Dynamics, 2018, 36, 3265-3273.	2.0	10
84	Fully Atomistic Multiscale Approach for pK_a Prediction. Journal of Physical Chemistry B, 2020, 124, 4712-4722.	1.2	10
85	Modeling amino-acid side chain infrared spectra: the case of carboxylic residues. Physical Chemistry Chemical Physics, 2020, 22, 3008-3016.	1.3	10
86	On the use of the quasi-Gaussian entropy theory in the study of simulated dilute solutions. Journal of Chemical Physics, 2004, 120, 5226-5234.	1.2	9
87	A Theoretical Model for the Folding/Unfolding Thermodynamics of Single-Domain Proteins, Based on the Quasi-Gaussian Entropy Theory. Journal of Physical Chemistry B, 2004, 108, 5756-5762.	1.2	9
88	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
89	In silico characterization of bimolecular electron transfer reactions: The ferroceneâ€“ferrocenium reaction as a test case. International Journal of Quantum Chemistry, 2016, 116, 1723-1730.	1.0	9
90	Theoretical-computational modeling of charge transfer and intersystem crossing reactions in complex chemical systems. RSC Advances, 2018, 8, 27900-27918.	1.7	9

#	Article	IF	Citations
91	Statistical Mechanical Modeling of Chemical Reactions in Condensed Phase Systems. Challenges and Advances in Computational Chemistry and Physics, 2008, , 191-213.	0.6	9
92	Theoretical Modeling of Redox Potentials of Biomolecules. Molecules, 2022, 27, 1077.	1.7	9
93	On the Use of the Quasi-Gaussian Entropy Theory in Systems of Polyatomic Flexible Molecules. Journal of Physical Chemistry B, 2001, 105, 1834-1844.	1.2	8
94	A fast redox-induced switching mechanism in a conformationally controllable molecular thread in solution. Physical Chemistry Chemical Physics, 2010, 12, 4552.	1.3	8
95	Effects of local electric fields on the redox free energy of single stranded DNA. Chemical Communications, 2011, 47, 2646-2648.	2.2	8
96	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
97	On the convergence of the conformational coordinates basis set obtained by the essential dynamics analysis of proteins' molecular dynamics simulations. , 1999, 36, 419.		8
98	Structural rearrangements of the two domains of Azotobacter vinelandii rhodanese upon sulfane sulfur release: essential molecular dynamics, NMR relaxation and deuterium exchange on the uniformly labeled protein. International Journal of Biological Macromolecules, 2003, 33, 193-201.	3.6	7
99	Myoglobin as a Case Study for Molecular Simulations in the Presence of a Microwave Electromagnetic Field. , 2006, , .		7
100	Intramolecular charge transfer in Ï€-conjugated oligomers: a theoretical study on the effect of temperature and oxidation state. Theoretical Chemistry Accounts, 2008, 119, 469-476.	0.5	7
101	Charge transfer equilibria of aqueous single stranded DNA. Physical Chemistry Chemical Physics, 2009, 11, 10614.	1.3	7
102	Free-Energy Profile for CO Binding to Separated Chains of Human and Trematomus newnesi Hemoglobin: Insights from Molecular Dynamics Simulations and Perturbed Matrix Method. Journal of Physical Chemistry B, 2010, 114, 7002-7008.	1.2	7
103	Entropyâ€“energy balance in base catalyzed ketoâ€enol interconversion: A joint theoretical and experimental investigation. International Journal of Quantum Chemistry, 2011, 111, 1293-1305.	1.0	7
104	Thermal and environmental effects on Oligothiophene low-energy singlet electronic excitations in dilute solution: a theoretical and experimental study. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	7
105	Conformational and Electronic Properties of a Microperoxidase in Aqueous Solution: A Computational Study. ChemPhysChem, 2005, 6, 681-689.	1.0	6
106	Ground and excited electronic state thermodynamics of aqueous carbon monoxide: A theoretical study. Journal of Chemical Physics, 2005, 122, 124507.	1.2	6
107	Modelling vibrational relaxation in complex molecular systems. Physical Chemistry Chemical Physics, 2019, 21, 20003-20017.	1.3	6
108	IR spectroscopy of condensed phase systems: Can the environment induce vibrational mode coupling?. Chemical Physics Letters, 2021, 763, 138168.	1.2	6

#	Article	IF	Citations
109	Stationary and Time-Dependent Carbon Monoxide Stretching Mode Features in Carboxy Myoglobin: A Theoreticalâ€“Computational Reappraisal. Journal of Physical Chemistry B, 2021, 125, 13624-13634.	1.2	6
110	Essential degrees of freedom of proteins. Molecular Engineering, 1995, 5, 71-79.	0.2	5
111	On the importance of configurational sampling in theoretical calculation of electronic properties of complex molecular systems: Acetone in water. Chemical Physics Letters, 2006, 424, 289-294.	1.2	5
112	On the catalytic role of structural fluctuations in enzyme reactions: computational evidence on the formation of compound 0 in horseradish peroxidase. Faraday Discussions, 0, 145, 107-119.	1.6	5
113	Inclusion of cybotactic effect in the theoretical modeling of absorption spectra of liquid-state systems with perturbed matrix method and molecular dynamics simulations: the UVâ€“Vis absorption spectrum of para-nitroaniline as a case study. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	5
114	Length-scale dependence of protein hydration-shell density. Physical Chemistry Chemical Physics, 2020, 22, 7340-7347.	1.3	5
115	The effects of the L29F mutation on the ligand migration kinetics in crystallized myoglobin as revealed by molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2011, 79, 867-879.	1.5	4
116	A theoretical study on the spectral and electrochemical properties of Ferrocene in different solvents. Inorganica Chimica Acta, 2013, 407, 82-90.	1.2	4
117	Theoreticalâ€“computational modelling of the temperature dependence of the foldingâ€“unfolding thermodynamics and kinetics: the case of a Trp-cage. Physical Chemistry Chemical Physics, 2019, 21, 23162-23168.	1.3	4
118	What can we learn by comparing experimental and theoretical-computational X-ray scattering data?. Journal of Molecular Liquids, 2009, 144, 9-12.	2.3	3
119	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
120	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
121	Theoretical-computational modelling of the L-alanine CD spectrum in water. Computational and Theoretical Chemistry, 2022, 1209, 113591.	1.1	3
122	Computational Modeling of the Thermodynamics of the Mesophilic and Thermophilic Mutants of Trp-Cage Miniprotein. ACS Omega, 2022, 7, 13448-13454.	1.6	3
123	Coherent dynamics in a butane molecule. Physical Review E, 2002, 66, 020901.	0.8	2
124	Characterization of liquid behaviour by means of local density fluctuations. Journal of Molecular Liquids, 2005, 117, 17-21.	2.3	2
125	Theoretical-computational modelling of the vibrational relaxation of small inorganic species in condensed phase. Results in Chemistry, 2022, 4, 100305.	0.9	2
126	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

#	Article	IF	Citations
127	Theoretical-computational characterization of the temperature-dependent folding thermodynamics of aÎ²-hairpin peptide. Chemical Physics Letters, 2016, 659, 247-251.	1.2	1
128	Evolutionary Modes in Protein Observable Space: The Case of Thioredoxins. Journal of Molecular Evolution, 2019, 87, 175-183.	0.8	1
129	On the convergence of the conformational coordinates basis set obtained by the essential dynamics analysis of proteins' molecular dynamics simulations. , 1999, 36, 419.		1
130	The role of water near charged interfaces: Molecular dynamics simulations of biological macromolecules in presence of high intense electric fields. , 2011, , .		0
131	Modeling electromagnetic field effects in a biochemical reaction: Understanding reactivity inhibition due to the magnetic field. , 2011, , .		0
132	Thermal and environmental effects on Oligothiophene low-energy singlet electronic excitations in dilute solution: a theoretical and experimental study. Highlights in Theoretical Chemistry, 2013, , 185-198.	0.0	0
133	The Perfect Enzyme : Revisiting the Modelling of Initial Proton Transfer in Triosephosphate Isomerase. Theoretical Biology Forum, 2016, 109, 13-36.	0.2	0