Riccardo Chelli

List of Publications by Year
in descending order

96 papers	2,841 citations	168829 31 h-index	214428 50 g-index
97 all docs	97 docs citations	97 times ranked	3146 citing authors

#	Article	IF	Citations
1	Ethanol electro-oxidation reaction on the Pd(111) surface in alkaline media: insights from quantum and molecular mechanics. Physical Chemistry Chemical Physics, 2022, , .	1.3	2
2	Polarizability relaxation in water/ethanol mixtures. Journal of Molecular Liquids, 2021, 332, 115839.	2.3	4
3	Imidazole in Aqueous Solution: Hydrogen Bond Interactions and Structural Reorganization with Concentration. Journal of Physical Chemistry B, 2019, 123, 4055-4064.	1.2	9
4	Computational Investigation of the Selective Cleavage of Diastereotopic Cyclopropane Bonds in 5-Spirocyclopropane Isoxazolidines Rearrangement. Journal of Organic Chemistry, 2019, 84, 6757-6764.	1.7	5
5	A Photochromic Azobenzene Peptidomimetic of a Î²-Turn Model Peptide Structure as a Conformational Switch. Frontiers in Chemistry, 2019, 7, 180.	1.8	9
6	Structural Insights into the Osteopontin-Aptamer Complex by Molecular Dynamics Simulations. Frontiers in Chemistry, 2018, 6, 2.	1.8	16
7	Correspondence between light-absorption spectrum and nonequilibrium work distribution as a mean to access free energy differences between electronic states. Journal of Chemical Physics, 2018, 149, 084101.	1.2	0
8	Photochemical Reactivity of 1,6-Methano[10]annulene. Journal of Physical Chemistry A, 2017, 121, 4412-4421.	1.1	2
9	Statistical Mechanics of Ligandâ€“Receptor Noncovalent Association, Revisited: Binding Site and Standard State Volumes in Modern Alchemical Theories. Journal of Chemical Theory and Computation, 2017, 13, 1924-1933.	2.3	39
10	Insights on the Realgar Crystal Under Pressure from XP-PCM and Periodic Model Calculations. Journal of Physical Chemistry A, 2017, 121, 8825-8834.	1.1	14
11	Binding Free Energies of Hostâ€“Guest Systems by Nonequilibrium Alchemical Simulations with Constrained Dynamics: Theoretical Framework. Journal of Chemical Theory and Computation, 2017, 13, 5874-5886.	2.3	14
12	Binding Free Energies of Hostâ€“Guest Systems by Nonequilibrium Alchemical Simulations with Constrained Dynamics: Illustrative Calculations and Numerical Validation. Journal of Chemical Theory and Computation, 2017, 13, 5887-5899.	2.3	14
13	Resolving capacity of infraredâ€“visible sum frequency generation microscopy to address discrete structural realizations of a protein at interface. Journal of Raman Spectroscopy, 2016, 47, 828-838.	1.2	1
14	Nonequilibrium work theorems applied to transitions between configurational domains. Journal of Statistical Mechanics: Theory and Experiment, 2016, 2016, 123204.	0.9	3
15	II. Dissociation free energies in drugâ€“receptor systems via nonequilibrium alchemical simulations: application to the FK506-related immunophilin ligands. Physical Chemistry Chemical Physics, 2016, 18, 15005-15018.	1.3	34
16	Elastic Barrier Dynamical Freezing in Free Energy Calculations: A Way To Speed Up Nonequilibrium Molecular Dynamics Simulations by Orders of Magnitude. Journal of Chemical Theory and Computation, 2016, 12, 1029-1039.	2.3	4
17	Simulations in generalized ensembles through noninstantaneous switches. Physical Review E, 2015, 92, 043310.	0.8	1
18	Computing Free Energy Differences of Configurational Basins. Journal of Chemical Theory and Computation, 2015, 11, 3561-3571.	2.3	5

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19	Polarization entanglement of sum-frequency photons: A tool to probe the Markovian limit. Physical Review A, 2015, 91, .	1.0	0
20	A fluorescent receptor for halide recognition: clues for the design of anion chemosensors. Physical Chemistry Chemical Physics, 2015, 17, 10813-10822.	1.3	11
21	Annealed importance sampling with constant cooling rate. Journal of Chemical Physics, 2015, 142, 074102.	1.2	1
22	Combining path-breaking with bidirectional nonequilibrium simulations to improve efficiency in free energy calculations. Journal of Chemical Physics, 2014, 140, 064104.	1.2	14
23	Nonequilibrium Candidate Monte Carlo Simulations with Configurational Freezing Schemes. Journal of Chemical Theory and Computation, 2014, 10, 4273-4283.	2.3	10
24	Convective Replica-Exchange in Ergodic Regimes. Journal of Chemical Theory and Computation, 2014, 10, 953-958.	2.3	3
25	Tuning the Emission Properties of Fluorescent Ligands by Changing pH: The Unusual Case of an Acridine-Containing Polyamine Macrocycle. Journal of Physical Chemistry A, 2013, 117, 3798-3808.	1.1	14
26	Toward quantitative estimates of binding affinities for proteinâ€“ligand systems involving large inhibitor compounds: A steered molecular dynamics simulation route. Journal of Computational Chemistry, 2013, 34, 1561-1576.	1.5	41
27	Path-breaking schemes for nonequilibrium free energy calculations. Journal of Chemical Physics, 2013, 138, 214109.	1.2	26
28	Local Sampling in Steered Monte Carlo Simulations Decreases Dissipation and Enhances Free Energy Estimates via Nonequilibrium Work Theorems. Journal of Chemical Theory and Computation, 2012, 8, 4040-4052.	2.3	26
29	Serial Generalized Ensemble Simulations of Biomolecules with Self-Consistent Determination of Weights. Journal of Chemical Theory and Computation, 2012, 8, 830-842.	2.3	17
30	Serial Generalized Ensemble Simulations of Biomolecules with Self-Consistent Determination of Weights. Journal of Chemical Theory and Computation, 2012, 8, 2552-2552.	2.3	5
31	Excitonic Effects in the 2DIR Spectra of Liquid Formamide. , 2012, , .		0
32	Excitonic effects in two-dimensional vibrational spectra of liquid formamide. Physical Chemistry Chemical Physics, 2011, 13, 11351.	1.3	5
33	Exploiting Configurational Freezing in Nonequilibrium Monte Carlo Simulations. Journal of Chemical Theory and Computation, 2011, 7, 582-593.	2.3	29
34	Structural Properties of a Membrane Associated Anchor Dipeptide. Journal of Physical Chemistry B, 2011, 115, 5294-5303.	1.2	12
35	ORAC: A molecular dynamics simulation program to explore free energy surfaces in biomolecular systems at the atomistic level. Journal of Computational Chemistry, 2010, 31, 1106-1116.	1.5	67
36	Hummer and Szabo-like Potential of Mean Force Estimator for Bidirectional Nonequilibrium Pulling Experiments/Simulations. Journal of Physical Chemistry B, 2010, 114, 9546-9554.	1.2	20

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37	Optimal Weights in Serial Generalized-Ensemble Simulations. Journal of Chemical Theory and Computation, 2010, 6, 1935-1950.	2.3	25
38	Two-dimensional infrared spectroscopy of a structured liquid: Neat formamide. Journal of Chemical Physics, 2009, 130, 204518.	1.2	11
39	Improving fast-switching free energy estimates by dynamical freezing. Physical Review E, 2009, 80, 041124.	0.8	17
40	Nonequilibrium work relations for systems subject to mechanical and thermal changes. Journal of Chemical Physics, 2009, 130, 054102.	1.2	17
41	A potential of mean force estimator based on nonequilibrium work exponential averages. Physical Chemistry Chemical Physics, 2009, 11, 1152.	1.3	37
42	Retrieval of spectral and dynamic properties from twoâ€dimensional infrared pumpâ€probe experiments. Journal of Computational Chemistry, 2008, 29, 1507-1516.	1.5	9
43	Polyamineâ^'Polycarboxylate Metal Complexes with Different Biological Effectiveness as Nitric Oxide Scavengers. Clues for Drug Design. Journal of Medicinal Chemistry, 2008, 51, 3250-3260.	2.9	11
44	Thermodynamics of stacking interactions in proteins. Physical Chemistry Chemical Physics, 2008, 10, 2673.	1.3	79
45	Approximating nonequilibrium processes using a collection of surrogate diffusion models. Journal of Chemical Physics, 2008, 128, 145103.	1.2	12
46	Calculation of the potential of mean force from nonequilibrium measurements via maximum likelihood estimators. Physical Review E, 2008, 77, 031104.	0.8	33
47	Electrostatic interactions in phospholipid membranes revealed by coherent 2D IR spectroscopy. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 15323-15327.	3.3	32
48	Numerical verification of the generalized Crooks nonequilibrium work theorem for non-Hamiltonian molecular dynamics simulations. Journal of Chemical Physics, 2007, 127, 034110.	1.2	15
49	Generalization of the Jarzynski and Crooks nonequilibrium work theorems in molecular dynamics simulations. Physical Review E, 2007, 75, 050101.	0.8	37
50	Key Role of the Polarization Anisotropy of Water in Modeling Classical Polarizable Force Fields. Journal of Physical Chemistry A, 2007, 111, 8170-8176.	1.1	76
51	Fluorescence Emissions and Torsional Conformations in Ï€-Conjugated Chains of PolyDCHD-HS. Journal of Physical Chemistry C, 2007, 111, 17485-17492.	1.5	4
52	Recovering the Crooks equation for dynamical systems in the isothermal-isobaric ensemble: A strategy based on the equations of motion. Journal of Chemical Physics, 2007, 126, 044502.	1.2	14
53	Problems in molecular dynamics of condensed phases. Theoretical Chemistry Accounts, 2007, 117, 1105-1120.	0.5	5
54	Free volume from molecular dynamics simulations and its relationships to the positron annihilation lifetime spectroscopy. Theoretical Chemistry Accounts, 2007, 118, 443-448.	0.5	9

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55	Self-healing Umbrella Sampling:Â A Non-equilibrium Approach for Quantitative Free Energy Calculations. Journal of Physical Chemistry B, 2006, 110, 14011-14013.	1.2	114
56	Metadynamics Simulation of Prion Protein:Â Î²-Structure Stability and the Early Stages of Misfolding. Journal of the American Chemical Society, 2006, 128, 2705-2710.	6.6	105
57	Domain Formation in Lipid Bilayers Probed by Two-Dimensional Infrared Spectroscopy. Journal of Physical Chemistry B, 2006, 110, 1499-1501.	1.2	19
58	Hydration and Hydrogen Bonding of Carbonyls in Dimyristoyl-Phosphatidylcholine Bilayer. Journal of the American Chemical Society, 2006, 128, 9466-9471.	6.6	34
59	Comment on â€œFrom Subtle to Substantial:Â Role of Metal Ions on Ï€â^'Ï€ Interactionsâ€• Journal of Physical Chemistry B, 2006, 110, 10204-10205.	1.2	9
60	Crooks equation for steered molecular dynamics using a NosÃ©-Hoover thermostat. Journal of Chemical Physics, 2006, 125, 164101.	1.2	60
61	1P216 Two-dimensional Infrared Spectroscopy and Molecular Dynamics of Liquid Formamide. Seibutsu Butsuri, 2005, 45, S85.	0.0	2
62	1P215 Domain formation in lipid bilayer probed in two-dimensional infrared ultrafast experiment. Seibutsu Butsuri, 2005, 45, S85.	0.0	0
63	Insights into positron annihilation lifetime spectroscopy by molecular dynamics simulations. European Physical Journal D, 2005, 32, 289-297.	0.6	17
64	Polarization response of water and methanol investigated by a polarizable force field and density functional theory calculations: Implications for charge transfer. Journal of Chemical Physics, 2005, 122, 074504.	1.2	40
65	Behavior of polarizable models in presence of strong electric fields. I. Origin of nonlinear effects in water point-charge systems. Journal of Chemical Physics, 2005, 123, 194109.	1.2	14
66	Comparing polarizable force fields to ab initio calculations reveals nonclassical effects in condensed phases. Journal of Chemical Physics, 2005, 122, 234107.	1.2	34
67	Structure of Liquid Formic Acid Investigated by First Principle and Classical Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2005, 109, 17006-17013.	1.2	25
68	Misfolding Pathways of the Prion Protein Probed by Molecular Dynamics Simulations. Biophysical Journal, 2005, 88, 1334-1343.	0.2	58
69	Dynamics of liquid benzene: A cage analysis. Journal of Chemical Physics, 2005, 123, 124511.	1.2	12
70	A study on the anisoleâ€“water complex by molecular beamâ€“electronic spectroscopy and molecular mechanics calculations. Journal of Chemical Physics, 2004, 120, 5601-5607.	1.2	47
71	Inter-residue and solvent-residue interactions in proteins: A statistical study on experimental structures. Proteins: Structure, Function and Bioinformatics, 2004, 55, 139-151.	1.5	15
72	Comment to â€œCalculation of the Dipole Moment for Polypeptides Using the Generalized Born-Electronegativity Equalization Method:Â Results in Vacuum and Continuum-Dielectric Solventâ€• Journal of Physical Chemistry B, 2004, 108, 16995-16997.	1.2	7

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73	Energetic Fitness of Histidine Protonation States in PDB Structures. Journal of Physical Chemistry B, 2004, 108, 12252-12257.	1.2	10
74	The Absorption Spectrum of Anisole and the Anisole/CO2 1:1-Cluster. The Influence of Intermolecular Interaction on Intramolecular Vibrations. Zeitschrift Fur Physikalische Chemie, 2004, 218, 123-154.	1.4	14
75	Dynamical and structural correlation in supercooled liquids: A molecular dynamics investigation of m-toluidine. Journal of Chemical Physics, 2003, 119, 357-363.	1.2	13
76	Comment on â€œClassical polarizable force fields parametrized from ab initio calculationsâ€•[J. Chem. Phys. 117, 1416 (2002)]. Journal of Chemical Physics, 2003, 118, 1571-1572.	1.2	6
77	Is the T-Shaped Toluene Dimer a Stable Intermolecular Complex?. Journal of Physical Chemistry A, 2002, 106, 2945-2948.	1.1	40
78	Molecular dynamics of glass-forming liquids: Structure and dynamics of liquid metatoluidine. Journal of Chemical Physics, 2002, 116, 6205-6215.	1.2	17
79	A transferable polarizable electrostatic force field for molecular mechanics based on the chemical potential equalization principle. Journal of Chemical Physics, 2002, 117, 9175-9189.	1.2	124
80	Stacking and T-shape Competition in Aromaticâ^'Aromatic Amino Acid Interactions. Journal of the American Chemical Society, 2002, 124, 6133-6143.	6.6	233
81	Towards a polarizable force field for molecular liquids. Journal of Molecular Liquids, 2002, 96-97, 87-100.	2.3	17
82	The nature of intermolecular interactions between aromatic amino acid residues. Proteins: Structure, Function and Bioinformatics, 2002, 48, 117-125.	1.5	72
83	The fast dynamics of benzene in the liquid phase. Part II. A molecular dynamics simulation. Physical Chemistry Chemical Physics, 2001, 3, 2803-2810.	1.3	53
84	The fast dynamics of benzene in the liquid phase. Part I. Optical Kerr effect experimental investigation. Physical Chemistry Chemical Physics, 2001, 3, 2795-2802.	1.3	60
85	Excited state photoelectron spectroscopy of anisoleDedicated to Professor F. DÃ¶rr on the occasion of his 80th birthday.. Physical Chemistry Chemical Physics, 2001, 3, 5358-5368.	1.3	28
86	Determination of the Potential of Mean Force of Aromatic Amino Acid Complexes in Various Solvents Using Molecular Dynamics Simulations:Â The Case of the Tryptophanâ^'Histidine Pair. Journal of Physical Chemistry B, 2001, 105, 7835-7846.	1.2	29
87	Density Functional Calculation of Structural and Vibrational Properties of Glycerol. Journal of Physical Chemistry A, 2000, 104, 5351-5357.	1.1	62
88	Conformational Distribution of Gas-phase Glycerol. Journal of Physical Chemistry A, 2000, 104, 11220-11222.	1.1	32
89	Simulated structure, dynamics, and vibrational spectra of liquid benzene. Journal of Chemical Physics, 2000, 113, 6851-6863.	1.2	65
90	Electrical response in chemical potential equalization schemes. Journal of Chemical Physics, 1999, 111, 8569-8575.	1.2	115

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91	Calculation of optical spectra in liquid methanol using molecular dynamics and the chemical potential equalization method. Journal of Chemical Physics, 1999, 111, 4218-4229.	1.2	66
92	Glycerol condensed phases Part I. A molecular dynamics study. Physical Chemistry Chemical Physics, 1999, 1, 871-877.	1.3	112
93	Glycerol condensed phases Part II.A molecular dynamics study of the conformational structure and hydrogen bonding. Physical Chemistry Chemical Physics, 1999, 1, 879-885.	1.3	126
94	A molecular dynamics study of translation-rotation coupling in the NaCN plastic crystal. Journal of Chemical Physics, 1997, 107, 8041-8050.	1.2	9
95	Calculation of elastic coherent neutron scattering spectra from molecular dynamics data: The NaCN plastic crystal. Chemical Physics Letters, 1997, 274, 335-340.	1.2	0
96	A molecular dynamics study of translation-rotation coupling in the NaCN plastic crystal. , 0, .		2