Michele Cascella

List of Publications by Year
in descending order

73 papers	2,209 citations	218592 26 h-index	243529 44 g-index
78 all docs	78 docs citations	78 times ranked	3056 citing authors

#	Article	IF	Citations
1	Coarse-Grained Model of Proteins Incorporating Atomistic Detail of the Active Site. Physical Review Letters, 2005, 95, 218102.	2.9	157
2	Microsolvation Effects on the Excited-State Dynamics of Protonated Tryptophan. Journal of the American Chemical Society, 2006, 128, 16938-16943.	6.6	144
3	Role of protein frame and solvent for the redox properties of azurin from Pseudomonas aeruginosa. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 19641-19646.	3.3	135
4	The Grignard Reaction â€“ Unraveling a Chemical Puzzle. Journal of the American Chemical Society, 2020, 142, 2984-2994.	6.6	84
5	Human infrared vision is triggered by two-photon chromophore isomerization. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, E5445-54.	3.3	80
6	AbÂInitioCalculation of Optical Spectra of Liquids: Many-Body Effects in the Electronic Excitations of Water. Physical Review Letters, 2006, 97, 137402.	2.9	77
7	Subtle Differences in Virus Composition Affect Disinfection Kinetics and Mechanisms. Applied and Environmental Microbiology, 2013, 79, 3455-3467.	1.4	76
8	Evolutionarily Conserved Functional Mechanics across Pepsin-like and Retroviral Aspartic Proteases. Journal of the American Chemical Society, 2005, 127, 3734-3742.	6.6	74
9	Formation of Boronate Ester Polymers with Efficient Intrastrand Chargeâ€Transfer Transitions by Threeâ€Component Reactions. European Journal of Inorganic Chemistry, 2007, 2007, 5177-5181.	1.0	68
10	A quinoxaline-fused tetrathiafulvalene-based sensitizer for efficient dye-sensitized solar cells. Chemical Communications, 2014, 50, 6540-6542.	2.2	65
11	How Solvent Dynamics Controls the Schlenk Equilibrium of Grignard Reagents: A Computational Study of CH‹sub›3‹/sub›MgCl in Tetrahydrofuran. Journal of Physical Chemistry B, 2017, 121, 4226-4237.	1.2	63
12	Formamide Hydrolysis Investigated by Multiple-Steering ab Initio Molecular Dynamics. Journal of Physical Chemistry B, 2004, 108, 369-375.	1.2	50
13	A Nonradial Coarse-Grained Potential for Proteins Produces Naturally Stable Secondary Structure Elements. Journal of Chemical Theory and Computation, 2010, 6, 315-324.	2.3	48
14	Dispersion state phase diagram of citrate-coated metallic nanoparticles in saline solutions. Nature Communications, 2020, 11, 5422.	5.8	47
15	Dynamics and energetics of water permeation through the aquaporin channel. Proteins: Structure, Function and Bioinformatics, 2004, 55, 924-931.	1.5	43
16	Recognition of Imipenem and Meropenem by the RND-Transporter MexB Studied by Computer Simulations. Journal of the American Chemical Society, 2012, 134, 19146-19158.	6.6	41
17	Supramolecular Packing Drives Morphological Transitions of Charged Surfactant Micelles. Angewandte Chemie - International Edition, 2020, 59, 18591-18598.	7.2	41
18	The Conformational Flexibility of the Carboxy Terminal Residues 105â”114 Is a Key Modulator of the Catalytic Activity and Stability of Macrophage Migration Inhibitory Factor. Biochemistry, 2008, 47, 10740-10756.	1.2	40

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19	Biomembrane solubilization mechanism by Triton X-100: a computational study of the three stage model. Physical Chemistry Chemical Physics, 2017, 19, 29780-29794.	1.3	39
20	Optical Spectra of Cu(II)â˜Azurin by Hybrid TDDFT-Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2007, 111, 10248-10252.	1.2	38
21	UV Radiation Induces Genomeâ€Mediated, Siteâ€Specific Cleavage in Viral Proteins. ChemBioChem, 2012, 13, 837-845.	1.3	37
22	Toward Chemically Resolved Computer Simulations of Dynamics and Remodeling of Biological Membranes. Journal of Physical Chemistry Letters, 2017, 8, 3586-3594.	2.1	35
23	Molecular Origin of Piezo- and Pyroelectric Properties in Collagen Investigated by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2012, 116, 1901-1907.	1.2	30
24	Electrostatic-Consistent Coarse-Grained Potentials for Molecular Simulations of Proteins. Journal of Chemical Theory and Computation, 2013, 9, 3515-3526.	2.3	29
25	Electrostatics and flexibility drive membrane recognition and early penetration by the antimicrobial peptide dendrimer bH1. Chemical Communications, 2013, 49, 8821.	2.2	29
26	Topologically Based Multipolar Reconstruction of Electrostatic Interactions in Multiscale Simulations of Proteins. Journal of Chemical Theory and Computation, 2008, 4, 1378-1385.	2.3	28
27	A Proficient Enzyme:Â Insights on the Mechanism of Orotidine Monophosphate Decarboxylase from Computer Simulations. Journal of the American Chemical Society, 2004, 126, 15730-15737.	6.6	26
28	Electronic tuning effects via cyano substitution of a fused tetrathiafulvaleneâ€“benzothiadiazole dyad for ambipolar transport properties. RSC Advances, 2014, 4, 2873-2878.	1.7	26
29	Excited state properties of liquid water. Journal of Physics Condensed Matter, 2009, 21, 033101.	0.7	24
30	Hybrid Particle-Field Model for Conformational Dynamics of Peptide Chains. Journal of Chemical Theory and Computation, 2018, 14, 1120-1130.	2.3	24
31	Hybrid Particle-Field Molecular Dynamics Simulations of Charged Amphiphiles in an Aqueous Environment. Journal of Chemical Theory and Computation, 2018, 14, 4928-4937.	2.3	23
32	Vibrational excitation in electron-CH4collisions: exchange interaction effects. Journal of Physics B: Atomic, Molecular and Optical Physics, 2001, 34, 705-723.	0.6	22
33	Structural insights on cholesterol endosynthesis: Binding of squalene and 2,3-oxidosqualene to supernatant protein factor. Journal of Structural Biology, 2015, 190, 261-270.	1.3	21
34	Self-assembled Î±-Tocopherol Transfer Protein Nanoparticles Promote Vitamin E Delivery Across an Endothelial Barrier. Scientific Reports, 2017, 7, 4970.	1.6	21
35	Multidrug Resistance and Efflux Pumps: Insights from Molecular Dynamics Simulations. Current Topics in Medicinal Chemistry, 2013, 13, 3165-3183.	1.0	21
36	On the Acceleration of Cu Electrodeposition by TBPS (3,3-thiobis-1-propanesulfonic acid): A Combined Electrochemical, STM, NMR, ESI-MS and DFT Study. Journal of the Electrochemical Society, 2013, 160, D3158-D3164.	1.3	18

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37	Four-component relativistic ³¹P NMR calculations for trans-platinum(<scp>ii</scp>) complexes: importance of the solvent and dynamics in spectral simulations. Dalton Transactions, 2019, 48, 8076-8083.	1.6	18
38	Mesoscale Electrostatics Driving Particle Dynamics in Nonhomogeneous Dielectrics. Journal of Chemical Theory and Computation, 2019, 15, 2033-2041.	2.3	17
39	Supramolecular Packing Drives Morphological Transitions of Charged Surfactant Micelles. Angewandte Chemie, 2020, 132, 18750-18757.	1.6	17
40	Optical properties of flavin mononucleotide: A QM/MM study of protein environment effects. Chemical Physics, 2011, 389, 35-38.	0.9	16
41	Multiple Steering Molecular Dynamics Applied to Water Exchange at Alkali Ions. Journal of Physical Chemistry B, 2002, 106, 13027-13032.	1.2	15
42	Challenges and Perspectives in Biomolecular Simulations: From the Atomistic Picture to Multiscale Modeling. Chimia, 2009, 63, 14.	0.3	15
43	Dispersion Corrected Atom-Centered Potentials for Phosphorus. Journal of Chemical Theory and Computation, 2009, 5, 2930-2934.	2.3	15
44	Human Cellular Retinaldehyde-Binding Protein Has Secondary Thermal 9-cis-Retinal Isomerase Activity. Journal of the American Chemical Society, 2014, 136, 137-146.	6.6	15
45	Hybrid particle-field molecular dynamics under constant pressure. Journal of Chemical Physics, 2020, 152, 184908.	1.2	15
46	Aggregation of Lipid A Variants: A Hybrid Particle-Field Model. Biochimica Et Biophysica Acta - General Subjects, 2021, 1865, 129570.	1.1	15
47	Electron-impact vibrational excitation of polyatomic gases: Exploratory calculations. Journal of Chemical Physics, 2001, 114, 1989-2000.	1.2	14
48	The influence of conformational fluctuations on enzymatic activity: modelling the functional motion of Î²-secretase. Journal of Physics Condensed Matter, 2005, 17, S1581-S1593.	0.7	14
49	Cis-retinoids and the chemistry of vision. Archives of Biochemistry and Biophysics, 2013, 539, 187-195.	1.4	14
50	Anthanthrene dye-sensitized solar cells: influence of the number of anchoring groups and substitution motif. RSC Advances, 2015, 5, 98643-98652.	1.7	14
51	Low Inhibiting Power of NÂ·Â·Â·CO Based Peptidomimetic Compounds against HIV-1 Protease: Insights from a QM/MM Study. Journal of Chemical Theory and Computation, 2010, 6, 1369-1379.	2.3	13
52	First-Principles Calculation of ¹H NMR Chemical Shifts of Complex Metal Polyhydrides: The Essential Inclusion of Relativity and Dynamics. Inorganic Chemistry, 2020, 59, 17509-17518.	1.9	12
53	Engineering Tocopherol Selectivity in Î±-TTP: A Combined In Vitro/In Silico Study. PLoS ONE, 2012, 7, e49195.	1.1	10
54	Mechanisms of recognition and binding of Î±-TTP to the plasma membrane by multi-scale molecular dynamics simulations. Frontiers in Molecular Biosciences, 2015, 2, 36.	1.6	10

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55	Mechanistic insights into formic acid dehydrogenation promoted by Cu-amino based systems. Inorganica Chimica Acta, 2018, 470, 290-294.	1.2	10
56	A fundamental catalytic difference between zinc and manganese dependent enzymes revealed in a bacterial isatin hydrolase. Scientific Reports, 2018, 8, 13104.	1.6	10
57	Toward accurate coarse-graining approaches for protein and membrane simulations. Chemical Modelling, 2015, , 1-52.	0.2	10
58	From Structure to Function: Characterization of Cu(I) Adducts in Leveler Additives by DFT Calculations. Journal of Physical Chemistry Letters, 2011, 2, 3081-3084.	2.1	9
59	Characterization of Molecular Determinants of the Conformational Stability of Macrophage Migration Inhibitory Factor: Leucine 46 Hydrophobic Pocket. PLoS ONE, 2012, 7, e45024.	1.1	9
60	Supramolecular Organization of Heptapyrenotide Oligomersâ€"An in Depth Investigation by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2013, 117, 2576-2585.	1.2	8
61	Intramolecular structural parameters are key modulators of the gel-liquid transition in coarse grained simulations of DPPC and DOPC lipid bilayers. Biochemical and Biophysical Research Communications, 2018, 498, 327-333.	1.0	8
62	Automated determination of hybrid particle-field parameters by machine learning. Molecular Physics, 2020, 118, e1785571.	0.8	8
63	Hamiltonian and alias-free hybrid particleâ€"field molecular dynamics. Journal of Chemical Physics, 2020, 153, 094106.	1.2	8
64	Can Polarity-Inverted Surfactants Self-Assemble in Nonpolar Solvents?. Journal of Physical Chemistry B, 2020, 124, 6448-6458.	1.2	8
65	Proton disorder in cubic ice: Effect on the electronic and optical properties. Journal of Chemical Physics, 2015, 143, 084507.	1.2	7
66	Cellular Retinaldehyde Binding Proteinâ€"Different Binding Modes and Micro-Solvation Patterns for High-Affinity 9-cis- and 11-cis-Retinal Substrates. Journal of Physical Chemistry B, 2013, 117, 10719-10729.	1.2	5
67	Self-Assembly of Î±-Tocopherol Transfer Protein Nanoparticles: A Patchy Protein Model. Journal of Physical Chemistry B, 2018, 122, 7066-7072.	1.2	5
68	Engineering of a functional Î³-tocopherol transfer protein. Redox Biology, 2021, 38, 101773.	3.9	5
69	Structural Origin of Metal Specificity in Isatin Hydrolase from Labrenzia aggregata Investigated by Computer Simulations. Chemistry - A European Journal, 2018, 24, 5074-5077.	1.7	4
70	Excited state properties of formamide in water solution: An ab initio study. Journal of Chemical Physics, 2012, 137, 164317.	1.2	2
71	Mechanisms of Ligandâ€"Protein Interaction in Sec-14-like Transporters Investigated by Computer Simulations. Chimia, 2014, 68, 615.	0.3	2
72	Wavefunction-Based Electrostatic-Embedding QM/MM Using CFOUR through MiMiC. Journal of Chemical Theory and Computation, 2022, 18, 13-24.	2.3	2

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73	Bias Amplification in Gender, Gender Identity, and Geographical Affiliation. Journal of Chemical Information and Modeling, 2022, , .	2.5	2