Marco Cecchini

List of Publications by Year
in descending order

47 papers	2,647 citations	270111 25 h-index	232693 48 g-index
54 all docs	54 docs citations	54 times ranked	4576 citing authors

#	Article	IF	Citations
1	TiO4N2 complexes formed with 1,10-phenanthroline ligands containing a donor-acceptor hydrogen bond site: synthesis, cytotoxicity and docking experiments. Inorganica Chimica Acta, 2022, , 121036.	1.2	1
2	Multibasin Quasi-Harmonic Approach for the Calculation of the Configurational Entropy of Small Molecules in Solution. Journal of Chemical Theory and Computation, 2021, 17, 1133-1142.	2.3	11
3	An Asymmetric Mechanism in a Symmetric Molecular Machine. Journal of Physical Chemistry Letters, 2021, 12, 3260-3265.	2.1	6
4	PrepFlow: A Toolkit for Chemical Library Preparation and Management for Virtual Screening. Molecular Informatics, 2021, 40, 2100139.	1.4	5
5	Nicotinic receptors: From protein allostery to computational neuropharmacology. Molecular Aspects of Medicine, 2021, 84, 101044.	2.7	10
6	On the Functional Annotation of Open-Channel Structures in the Glycine Receptor. Structure, 2020, 28, 690-693.e3.	1.6	9
7	The Glycine Receptor Allosteric Ligands Library (GRALL). Bioinformatics, 2020, 36, 3379-3384.	1.8	21
8	Allostery in Its Many Disguises: From Theory to Applications. Structure, 2019, 27, 566-578.	1.6	285
9	Harnessing complexity in molecular self-assembly using computer simulations. Physical Chemistry Chemical Physics, 2018, 20, 6767-6776.	1.3	15
10	Modeling the adsorption equilibrium of small-molecule gases on graphene: effect of the volume to surface ratio. Physical Chemistry Chemical Physics, 2018, 20, 9770-9779.	1.3	3
11	An Ion-Permeable State of the Glycine Receptor Captured by Molecular Dynamics. Structure, 2018, 26, 1555-1562.e4.	1.6	34
12	An intermediate along the recovery stroke of myosin VI revealed by X-ray crystallography and molecular dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 6213-6218.	3.3	22
13	A Linear Interaction Energy Model for Cavitand Hostâ€“Guest Binding Affinities. Journal of Physical Chemistry B, 2018, 122, 6810-6814.	1.2	5
14	On the permeation of large organic cations through the pore of ATP-gated P2X receptors. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E3786-E3795.	3.3	79
15	Un-gating and allosteric modulation of a pentameric ligand-gated ion channel captured by molecular dynamics. PLoS Computational Biology, 2017, 13, e1005784.	1.5	32
16	Photo-switchable tweezers illuminate pore-opening motions of an ATP-gated P2X ion channel. ELife, 2016, 5, e11050.	2.8	31
17	Perchlorination of Coronene Enhances its Propensity for Selfâ€Assembly on Graphene. ChemPhysChem, 2016, 17, 330-330.	1.0	1
18	Perchlorination of Coronene Enhances its Propensity for Selfâ€Assembly on Graphene. ChemPhysChem, 2016, 17, 352-357.	1.0	24

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19	Myosin MyTH4-FERM structures highlight important principles of convergent evolution. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E2906-15.	3.3	20
20	Computational Approaches to the Chemical Equilibrium Constant in Proteinâ€ligand Binding. Molecular Informatics, 2016, 35, 555-567.	1.4	16
21	Predicting molecular self-assembly at surfaces: a statistical thermodynamics and modeling approach. Physical Chemistry Chemical Physics, 2016, 18, 31480-31493.	1.3	33
22	Atomically Precise Prediction of 2D Selfâ€Assembly of Weakly Bonded Nanostructures: STM Insight into Concentrationâ€Dependent Architectures. Small, 2016, 12, 343-350.	5.2	33
23	Space and Time Evolution of the Electrostatic Potential During the Activation of a Visual Pigment. Journal of Physical Chemistry Letters, 2016, 7, 2563-2567.	2.1	8
24	Surfaceâ€Induced Selection During Inâ€...Situ Photoswitching at the Solid/Liquid Interface. Angewandte Chemie - International Edition, 2015, 54, 4865-4869.	7.2	48
25	The nicotinic acetylcholine receptor and its prokaryotic homologues: Structure, conformational transitions & allosteric modulation. Neuropharmacology, 2015, 96, 137-149.	2.0	113
26	Accurate Calculation of Conformational Free Energy Differences in Explicit Water: The Confinementâ€“Solvation Free Energy Approach. Journal of Physical Chemistry B, 2015, 119, 5194-5207.	1.2	19
27	Quantum Corrections to the Free Energy Difference between Peptides and Proteins Conformers. Journal of Chemical Theory and Computation, 2015, 11, 4011-4022.	2.3	4
28	Accurate and Efficient Calculation of the Desorption Energy of Small Molecules from Graphene. Journal of Physical Chemistry C, 2015, 119, 1867-1879.	1.5	26
29	A Supramolecular Strategy to Leverage the Liquidâ€Phase Exfoliation of Graphene in the Presence of Surfactants: Unraveling the Role of the Length of Fatty Acids. Small, 2015, 11, 1691-1702.	5.2	87
30	Allosteric regulation of pentameric ligand-gated ion channels: An emerging mechanistic perspective. Channels, 2014, 8, 350-360.	1.5	31
31	A Simplified Confinement Method for Calculating Absolute Free Energies and Free Energy and Entropy Differences. Journal of Physical Chemistry B, 2013, 117, 750-762.	1.2	30
32	A gating mechanism of pentameric ligand-gated ion channels. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, E3987-96.	3.3	129
33	Predicting self-assembly: from empirism to determinism. Chemical Society Reviews, 2012, 41, 3713.	18.7	179
34	A Conformational Transition in the Myosin VI Converter Contributes to the Variable Step Size. Biophysical Journal, 2011, 101, 2436-2444.	0.2	17
35	Self-templating 2D supramolecular networks: a new avenue to reach control over a bilayer formation. Nanoscale, 2011, 3, 4125.	2.8	46
36	Adsorption of Aromatic and Anti-Aromatic Systems on Graphene through Ï€â^Ï€ Stacking. Journal of Physical Chemistry Letters, 2010, 1, 3407-3412.	2.1	344

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37	Pi Release from Myosin: A Simulation Analysis of Possible Pathways. Structure, 2010, 18, 458-470.	1.6	50
38	Conformational Free-Energy Difference of a Miniprotein from Nonequilibrium Simulations. Journal of Physical Chemistry Letters, 2010, 1, 1922-1926.	2.1	17
39	Atomistic Simulations of 2D Bicomponent Self-Assembly: From Molecular Recognition to Self-Healing. Journal of the American Chemical Society, 2010, 132, 17880-17885.	6.6	76
40	Calculation of Free-Energy Differences by Confinement Simulations. Application to Peptide Conformers. Journal of Physical Chemistry B, 2009, 113, 9728-9740.	1.2	47
41	Allosteric Communication in Myosin V: From Small Conformational Changes to Large Directed Movements. PLoS Computational Biology, 2008, 4, e1000129.	1.5	81
42	Wordom: a program for efficient analysis of molecular dynamics simulations. Bioinformatics, 2007, 23, 2625-2627.	1.8	251
43	In Silico Discovery of Î²-Secretase Inhibitors. Journal of the American Chemical Society, 2006, 128, 5436-5443.	6.6	93
44	A Molecular Dynamics Approach to the Structural Characterization of Amyloid Aggregation. Journal of Molecular Biology, 2006, 357, 1306-1321.	2.0	85
45	Discovery of Cell-Permeable Non-Peptide Inhibitors of Î²-Secretase by High-Throughput Docking and Continuum Electrostatics Calculations#. Journal of Medicinal Chemistry, 2005, 48, 5108-5111.	2.9	90
46	Automated docking of highly flexible ligands by genetic algorithms: A critical assessment. Journal of Computational Chemistry, 2004, 25, 412-422.	1.5	56
47	A Monte Carlo study of the chiral columnar organizations of dissymmetric discotic mesogens. Journal of Chemical Physics, 2003, 119, 9933-9946.	1.2	17