Walter Rocchia

List of Publications by Year
in descending order

75 papers	3,834 citations	186265 28 h-index	128289 60 g-index
83 all docs	83 docs citations	83 times ranked	4797 citing authors

#	ARTICLE	IF	CITATIONS
1	Extending the Applicability of the Nonlinear Poissonâˇ˜Boltzmann Equation:Â Multiple Dielectric Constants and Multivalent Ionsâ€. Journal of Physical Chemistry B, 2001, 105, 6507-6514.	2.6	747
2	Rapid grid-based construction of the molecular surface and the use of induced surface charge to calculate reaction field energies: Applications to the molecular systems and geometric objects. Journal of Computational Chemistry, 2002, 23, 128-137.	3.3	631
3	Wearable, Redundant Fabric-Based Sensor Arrays for Reconstruction of Body Segment Posture. IEEE Sensors Journal, 2004, 4, 807-818.	4.7	221
4	A catalytically silent FAAH-1 variant drives anandamide transport in neurons. Nature Neuroscience, 2012, 15, 64-69.	14.8	150
5	Steered Molecular Dynamics Simulations for Studying Proteinâ€"Ligand Interaction in Cyclin-Dependent Kinase 5. Journal of Chemical Information and Modeling, 2014, 54, 470-480.	5.4	138
6	Kinetics of protein-ligand unbinding via smoothed potential molecular dynamics simulations. Scientific Reports, 2015, 5, 11539.	3.3	132
7	Analytical electrostatics for biomolecules: Beyond the generalizedâ€‡ Born approximation. Journal of Chemical Physics, 2006, 124, 124902.	3.0	113
8	Kinetics of Drug Binding and Residence Time. Annual Review of Physical Chemistry, 2019, 70, 143-171.	10.8	105
9	A general and Robust Ray-Casting-Based Algorithm for Triangulating Surfaces at the Nanoscale. PLoS ONE, 2013, 8, e59744.	2.5	98
10	The ligand binding mechanism to purine nucleoside phosphorylase elucidated via molecular dynamics and machine learning. Nature Communications, 2015, 6, 6155.	12.8	98
11	Systematic Exploitation of Multiple Receptor Conformations for Virtual Ligand Screening. PLoS ONE, 2011, 6, e18845.	2.5	82
12	Multiplexed Discrimination of Single Amino Acid Residues in Polypeptides in a Single SERS Hot Spot. Angewandte Chemie - International Edition, 2020, 59, 11423-11431.	13.8	71
13	dMM-PBSA: A New HADDOCK Scoring Function for Protein-Peptide Docking. Frontiers in Molecular Biosciences, 2016, 3, 46.	3.5	67
14	A Pipeline To Enhance Ligand Virtual Screening: Integrating Molecular Dynamics and Fingerprints for Ligand and Proteins. Journal of Chemical Information and Modeling, 2015, 55, 2256-2274.	5.4	65
15	Mapping All-Atom Models onto One-Bead Coarse-Grained Models:Â General Properties and Applications to a Minimal Polypeptide Model. Journal of Chemical Theory and Computation, 2006, 2, 667-673.	5.3	64
16	Green Fluorescent Protein Ground States:â€‰ The Influence of a Second Protonation Site near the Chromophore,. Biochemistry, 2007, 46, 5494-5504.	2.5	60
17	Kinetic and Structural Insights into the Mechanism of Binding of Sulfonamides to Human Carbonic Anhydrase by Computational and Experimental Studies. Journal of Medicinal Chemistry, 2016, 59, 4245-4256.	6.4	60
18	Allosteric Communication Networks in Proteins Revealed through Pocket Crosstalk Analysis. ACS Central Science, 2017, 3, 949-960.	11.3	60

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19	DelPhi Web Server: A Comprehensive Online Suite for Electrostatic Calculations of Biological Macromolecules and Their Complexes. Communications in Computational Physics, 2013, 13, 269-284.	1.7	52
20	BiKi Life Sciences: A New Suite for Molecular Dynamics and Related Methods in Drug Discovery. Journal of Chemical Information and Modeling, 2018, 58, 219-224.	5.4	48
21	Between Algorithm and Model: Different Molecular Surface Definitions for the Poisson-Boltzmann Based Electrostatic Characterization of Biomolecules in Solution. Communications in Computational Physics, 2013, 13, 61-89.	1.7	46
22	Implicit solvent methods for free energy estimation. European Journal of Medicinal Chemistry, 2015, 91, 27-42.	5.5	46
23	AClAP, Autonomous hierarchical agglomerative Cluster Analysis based protocol to partition conformational datasets. Bioinformatics, 2006, 22, e58-e65.	4.1	41
24	Fast Dynamic Docking Guided by Adaptive Electrostatic Bias: The MD-Binding Approach. Journal of Chemical Theory and Computation, 2018, 14, 1727-1736.	5.3	40
25	Force Field Parametrization of Metal Ions from Statistical Learning Techniques. Journal of Chemical Theory and Computation, 2018, 14, 255-273.	5.3	39
26	Binding and Internalization in Receptor–Targeted Carriers: The Complex Role of CD44 in the Uptake of Hyaluronic Acid–Based Nanoparticles (siRNA Delivery). Advanced Healthcare Materials, 2019, 8, e1901182.	7.6	37
27	PypKa: A Flexible Python Module for Poisson–Boltzmann-Based pK_a Calculations. Journal of Chemical Information and Modeling, 2020, 60, 4442-4448.	5.4	33
28	JavaProtein Dossier: a novel web-based data visualization tool for comprehensive analysis of protein structure. Nucleic Acids Research, 2004, 32, W595-W601.	14.5	30
29	Complexes of HIV–1 integrase with HAT proteins: Multiscale models, dynamics, and hypotheses on allosteric sites of inhibition. Proteins: Structure, Function and Bioinformatics, 2009, 76, 946-958.	2.6	29
30	Shape-dependent effects of dielectrically nonlinear inclusions in heterogeneous media. Journal of Applied Physics, 2005, 98, 104101.	2.5	27
31	Using DelPhi Capabilities to Mimic Protein's Conformational Reorganization with Amino Acid Specific Dielectric Constants. Communications in Computational Physics, 2013, 13, 13-30.	1.7	23
32	NanoShaper–VMD interface: computing and visualizing surfaces, pockets and channels in molecular systems. Bioinformatics, 2019, 35, 1241-1243.	4.1	23
33	Pandemic drugs at pandemic speed: infrastructure for accelerating COVID-19 drug discovery with hybrid machine learning- and physics-based simulations on high-performance computers. Interface Focus, 2021, 11, 20210018.	3.0	23
34	Chromatin Compaction Multiscale Modeling: A Complex Synergy Between Theory, Simulation, and Experiment. Frontiers in Molecular Biosciences, 2020, 7, 15.	3.5	21
35	Probing Hydration Patterns in Class-A GPCRs via Biased MD: The A_{2A} Receptor. Journal of Chemical Theory and Computation, 2016, 12, 6049-6061.	5.3	18
36	FACE: facial automaton for conveying emotions. Applied Bionics and Biomechanics, 2004, 1, 91-100.	1.1	16

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37	Poisson-boltzmann equation boundary conditions for biological applications. Mathematical and Computer Modelling, 2005, 41, 1109-1118.	2.0	15
38	Finding Principal Paths in Data Space. IEEE Transactions on Neural Networks and Learning Systems, 2019, 30, 2449-2462.	11.3	15
39	Insights into Ligand–Protein Binding from Local Mechanical Response. Journal of Chemical Theory and Computation, 2011, 7, 3368-3378.	5.3	14
40	Molecular mechanics and dynamics: numerical tools to sample the configuration space. Frontiers in Bioscience - Landmark, 2014, 19, 578.	3.0	13
41	Predicting the dielectric nonlinearity of anisotropic composite materials via tensorial analysis. Journal of Physics Condensed Matter, 2006, 18, 10585-10599.	1.8	12
42	A simple and accurate protocol for absolute polar metabolite quantification in cell cultures using quantitative nuclear magnetic resonance. Analytical Biochemistry, 2016, 501, 26-34.	2.4	12
43	Electroactive carbon nanotube actuators: Soft-lithographic fabrication and electro-chemical modelling. Materials Science and Engineering C, 2008, 28, 1057-1064.	7.3	11
44	Import Vector Domain Description: A Kernel Logistic One-Class Learning Algorithm. IEEE Transactions on Neural Networks and Learning Systems, 2017, 28, 1722-1729.	11.3	11
45	The role of histone tails in nucleosome stability: An electrostatic perspective. Computational and Structural Biotechnology Journal, 2020, 18, 2799-2809.	4.1	11
46	Charged dielectric spheres interacting in electrolytic solution: A linearized Poisson–Boltzmann equation model. Journal of Chemical Physics, 2021, 155, 114114.	3.0	11
47	Enhanced Sampling Methods in Drug Design. RSC Drug Discovery Series, 2012, , 273-301.	0.3	11
48	A Fast and Interpretable Deep Learning Approach for Accurate Electrostatics-Driven pK_a Predictions in Proteins. Journal of Chemical Theory and Computation, 2022, 18, 5068-5078.	5.3	11
49	Describing the Conformational Landscape of Small Organic Molecules through Gaussian Mixtures in Dihedral Space. Journal of Chemical Theory and Computation, 2014, 10, 2557-2568.	5.3	10
50	SHREC 2021: Retrieval and classification of protein surfaces equipped with physical and chemical properties. Computers and Graphics, 2021, 99, 1-21.	2.5	10
51	SHREC 2022: Protein–ligand binding site recognition. Computers and Graphics, 2022, 107, 20-31.	2.5	10
52	A Combined MPI-CUDA Parallel Solution of Linear and Nonlinear Poisson-Boltzmann Equation. BioMed Research International, 2014, 2014, 1-12.	1.9	9
53	GPU linear and non-linear Poisson–Boltzmann solver module for DelPhi. Bioinformatics, 2014, 30, 569-570.	4.1	9
54	Adaptive nanopores: A bioinspired label-free approach for protein sequencing and identification. Nano Research, 2021, 14, 328-333.	10.4	9

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55	Cognitive Insights into Sentic Spaces Using Principal Paths. Cognitive Computation, 2019, 11, 656-675.	5.2	8
56	Antibody-Antigen Binding Interface Analysis in the Big Data Era. Frontiers in Molecular Biosciences, 0, 9, .	3.5	8
57	Application of Conformational Clustering in Protein–Ligand Docking. Methods in Molecular Biology, 2012, 819, 169-186.	0.9	7
58	Enhanced Molecular Dynamics Method to Efficiently Increase the Discrimination Capability of Computational Protein–Protein Docking. Journal of Chemical Theory and Computation, 2021, 17, 7271-7280.	5.3	6
59	Strain-amplified electroactive polymer actuator for haptic interfaces. , 2001, , .		5
60	Tuning Local Hydration Enables a Deeper Understanding of Protein–Ligand Binding: The PP1-Src Kinase Case. Journal of Physical Chemistry Letters, 2021, 12, 49-58.	4.6	5
61	Molecular Recognition by Gold Nanoparticle-Based Receptors as Defined through Surface Morphology and Pockets Fingerprint. Journal of Physical Chemistry Letters, 2021, 12, 5616-5622.	4.6	5
62	CUDA Accelerated Blobby Molecular Surface Generation. Lecture Notes in Computer Science, 2012, , 347-356.	1.3	5
63	CUDA accelerated molecular surface generation. Concurrency Computation Practice and Experience, 2014, 26, 1819-1831.	2.2	4
64	Absolute nutrient concentration measurements in cell culture media: 1H q-NMR spectra and data to compare the efficiency of pH-controlled protein precipitation versus CPMG or post-processing filtering approaches. Data in Brief, 2016, 8, 387-393.	1.0	3
65	Distributed Kernel K-Means for Large Scale Clustering. , 2017, , .		3
66	SDPhound, a Mutual Information-Based Method to Investigate Specificity-Determining Positions. Algorithms, 2009, 2, 764-789.	2.1	2
67	Solving the Linearized Poisson-Boltzmann Equation on GPUs Using CUDA. , 2013, , .		2
68	Including diverging electrostatic potential in 3D-RISM theory: The charged wall case. Journal of Chemical Physics, 2018, 148, 114106.	3.0	2
69	The State of the Science for the Langevin-Lorentz Model. , 1999, , 375-378.		2
70	Exploiting conducting polymer fiber radial expansion for bio-inspired actuation. , 2003, , .		1
71	Specific Residue Interactions Regulate the Binding of Dengue Antigens to Broadly Neutralizing EDE Antibodies. ChemistryOpen, 2018, 7, 604-610.	1.9	1
72	Building and Analyzing Molecular Surfaces: A Tutorial on NanoShaper. , 2015, , 199-213.		1

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73	Combined atomistic and continuum methods to map electric properties of nanostructured carbon films. Computational Materials Science, 2004, 30, 150-154.	3.0	0
74	A statistical mechanics handbook for protein-ligand binding simulation. Frontiers in Bioscience - Scholar, 2013, S5, 478-495.	2.1	0
75	ASSEMBLING GOLD NANOPARTICLE PATTERNS FOR MOLECULAR ELECTRONICS APPLICATIONS. , 2000, , .		0