Christopher N Rowley

List of Publications by Year
in descending order

57 papers	3,300 citations	172457 29 h-index	144013 57 g-index
94 all docs	94 docs citations	94 times ranked	4298 citing authors

#	Article	IF	Citations
1	Interaction between Antimicrobial Peptide Magainin 2 and Nonlipid Components in the Bacterial Outer Envelope. Journal of Physical Chemistry B, 2022, 126, 5473-5480.	2.6	2
2	Measuring and predicting warhead and residue reactivity. Annual Reports in Medicinal Chemistry, 2021, 56, 203-227.	0.9	2
3	Modeling the Binding and Conformational Energetics of a Targeted Covalent Inhibitor to Bruton's Tyrosine Kinase. Journal of Chemical Information and Modeling, 2021, 61, 5234-5242.	5.4	12
4	Unlocking the Friedel-Crafts arylation of primary aliphatic alcohols and epoxides driven by hexafluoroisopropanol. CheM, 2021, 7, 3425-3441.	11.7	44
5	Quantum Chemical Methods for Modeling Covalent Modification of Biological Thiols. Journal of Computational Chemistry, 2020, 41, 427-438.	3.3	31
6	Benchmarking Force Field and the ANI Neural Network Potentials for the Torsional Potential Energy Surface of Biaryl Drug Fragments. Journal of Chemical Information and Modeling, 2020, 60, 6258-6268.	5.4	15
7	Flexible Fitting of Small Molecules into Electron Microscopy Maps Using Molecular Dynamics Simulations with Neural Network Potentials. Journal of Chemical Information and Modeling, 2020, 60, 2591-2604.	5.4	24
8	Polarisable force fields: what do they add in biomolecular simulations?. Current Opinion in Structural Biology, 2020, 61, 182-190.	5.7	63
9	Simulating protein–ligand binding with neural network potentials. Chemical Science, 2020, 11, 2362-2368.	7.4	51
10	An efficient and accurate model for water with an improved non-bonded potential. Journal of Chemical Physics, 2020, 153, 134105.	3.0	3
11	$C(sp^3)$–$C(sp^3)$ Coupling with a Pd(II) Complex Bearing a Structurally Responsive Ligand. Organometallics, 2019, 38, 1677-1681.	2.3	4
12	Mechanisms of Alkyl and Aryl Thiol Addition to *N*-Methylmaleimide. Journal of Organic Chemistry, 2018, 83, 11674-11685.	3.2	14
13	Ring-opening hydroarylation of monosubstituted cyclopropanes enabled by hexafluoroisopropanol. Chemical Science, 2018, 9, 6411-6416.	7.4	62
14	The hydration structure of methylthiolate from QM/MM molecular dynamics. Journal of Chemical Physics, 2018, 149, 045103.	3.0	18
15	How Reactive are Druggable Cysteines in Protein Kinases?. Journal of Chemical Information and Modeling, 2018, 58, 1935-1946.	5.4	44
16	Evaluating the London Dispersion Coefficients of Protein Force Fields Using the Exchange-Hole Dipole Moment Model. Journal of Physical Chemistry B, 2018, 122, 6690-6701.	2.6	32
17	Folding free energy landscapes of *β*-sheets with non-polarizable and polarizable CHARMM force fields. Journal of Chemical Physics, 2018, 149, 072317.	3.0	28
18	Simulations of lipid bilayers using the CHARMM36 force field with the TIP3P-FB and TIP4P-FB water models. PeerJ, 2018, 6, e5472.	2.0	23

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19	Modeling covalent-modifier drugs. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2017, 1865, 1664-1675.	2.3	67
20	Evaluating Force-Field London Dispersion Coefficients Using the Exchange-Hole Dipole Moment Model. Journal of Chemical Theory and Computation, 2017, 13, 6146-6157.	5.3	40
21	The hydration structure of carbon monoxide byab initiomethods. Journal of Chemical Physics, 2017, 146, 034503.	3.0	5
22	An explicit-solvent conformation search method using open software. PeerJ, 2016, 4, e2088.	2.0	6
23	Simulation-Based Approaches for Determining Membrane Permeability of Small Compounds. Journal of Chemical Information and Modeling, 2016, 56, 721-733.	5.4	174
24	Evaluation of Methods for the Calculation of the pK_a of Cysteine Residues in Proteins. Journal of Chemical Theory and Computation, 2016, 12, 4662-4673.	5.3	88
25	Generalized Langevin Methods for Calculating Transmembrane Diffusivity. Journal of Chemical Theory and Computation, 2016, 12, 5609-5619.	5.3	42
26	Molecular simulation of nonfacilitated membrane permeation. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1672-1687.	2.6	114
27	Polarizable Force Field with a σ-Hole for Liquid and Aqueous Bromomethane. Journal of Physical Chemistry B, 2015, 119, 13422-13432.	2.6	17
28	Automated computational screening of the thiol reactivity of substituted alkenes. Journal of Computer-Aided Molecular Design, 2015, 29, 725-735.	2.9	19
29	The CHARMM–TURBOMOLE interface for efficient and accurate QM/MM molecular dynamics, free energies, and excited state properties. Journal of Computational Chemistry, 2014, 35, 2076-2086.	3.3	51
30	Combined Experimental and Computational Studies on the Physical and Chemical Properties of the Renewable Amide, 3â€Acetamidoâ€5â€acetylfuran. ChemPhysChem, 2014, 15, 4087-4094.	2.1	28
31	Solvation of Hydrogen Sulfide in Liquid Water and at the Water–Vapor Interface Using a Polarizable Force Field. Journal of Physical Chemistry B, 2014, 118, 1373-1380.	2.6	31
32	Why Can Hydrogen Sulfide Permeate Cell Membranes?. Journal of the American Chemical Society, 2014, 136, 15111-15113.	13.7	90
33	The tipping point of the inert pair effect: experimental and computational comparison of In(i) and Sn(ii) bis(imino)pyridine complexes. Dalton Transactions, 2014, 43, 690-697.	3.3	24
34	Benchmarking Quantum Chemical Methods for the Calculation of Molecular Dipole Moments and Polarizabilities. Journal of Physical Chemistry A, 2014, 118, 3678-3687.	2.5	205
35	Range-Separated DFT Functionals are Necessary to Model Thio-Michael Additions. Journal of Chemical Theory and Computation, 2013, 9, 4860-4865.	5.3	67
36	A Drude Polarizable Model for Liquid Hydrogen Sulfide. Journal of Physical Chemistry B, 2013, 117, 5222-5229.	2.6	20

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37	QM/MM molecular dynamics simulations of the hydration of Mg(II) and Zn(II) ions. Canadian Journal of Chemistry, 2013, 91, 552-558.	1.1	36
38	A computational study of barium blockades in the KcsA potassium channel based on multi-ion potential of mean force calculations and free energy perturbation. Journal of General Physiology, 2013, 142, 451-463.	1.9	16
39	Importance of Secondary Interactions in Twisted Doubly Hydrogen Bonded Complexes. Organic Letters, 2012, 14, 5772-5775.	4.6	1
40	The Solvation Structure of Na^+ and K^+ in Liquid Water Determined from High Level *ab Initio* Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2012, 8, 3526-3535.	5.3	191
41	Counteranion Effects on the Zirconocene Polymerization Catalyst Olefin Complex from QM/MM Molecular Dynamics Simulations. Organometallics, 2011, 30, 2071-2074.	2.3	37
42	Ion selectivity in channels and transporters. Journal of General Physiology, 2011, 137, 415-426.	1.9	142
43	New shooting algorithms for transition path sampling: Centering moves and varied-perturbation sizes for improved sampling. Journal of Chemical Physics, 2009, 131, 234102.	3.0	6
44	A Computational Experiment of the Endo versus Exo Preference in a Diels–Alder Reaction. Journal of Chemical Education, 2009, 86, 199.	2.3	22
45	Solution Conformation of C-Linked Antifreeze Glycoprotein Analogues and Modulation of Ice Recrystallization. Journal of the American Chemical Society, 2009, 131, 15745-15753.	13.7	56
46	Atom efficient cyclotrimerization of dimethylcyanamide catalyzed by aluminium amide: a combined experimental and theoretical investigation. Chemical Communications, 2008, , 3645.	4.1	21
47	Reaction Dynamics of β-Hydrogen Transfer in the Zirconocene Olefin Polymerization Catalyst: A DFT Path Sampling Study. Organometallics, 2008, 27, 6405-6407.	2.3	16
48	Mechanism of Olefin Hydrogenation Catalyzed by $RuHCl(L)(PR_3)_2$ Complexes (L) Tj ETQq0 0 0 rgBT /Overlock	2.3	22
49	A Path Sampling Study of Ru-Hydride-Catalyzed H2 Hydrogenation of Ethylene. Journal of the American Chemical Society, 2008, 130, 7218-7219.	13.7	22
50	Analysis of the Critical Step in Catalytic Carbodiimide Transformation: Proton Transfer from Amines, Phosphines, and Alkynes to Guanidinates, Phosphaguanidinates, and Propiolamidinates with Li and Al Catalysts. Inorganic Chemistry, 2008, 47, 12024-12031.	4.0	27
51	DFT Study of the Isomerization and Spectroscopic/Structural Properties of Ruthenacyclobutane Intermediates Relevant to Olefin Metathesis. Organometallics, 2008, 27, 6043-6045.	2.3	42
52	Amidolithium and Amidoaluminum Catalyzed Synthesis of Substituted Guanidines: An Interplay of DFT Modeling and Experiment. Inorganic Chemistry, 2008, 47, 9660-9668.	4.0	39
53	Generation of initial trajectories for transition path sampling of chemical reactions with ab initio molecular dynamics. Journal of Chemical Physics, 2007, 126, 024110.	3.0	12
54	Catalytic Intermolecular Direct Arylation of Perfluorobenzenes. Journal of the American Chemical Society, 2006, 128, 8754-8756.	13.7	801

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55	Synthesis and Thermolysis of Aluminum Amidinates: A Ligand-Exchange Route for New Mixed-Ligand Systems. Inorganic Chemistry, 2006, 45, 2276-2281.	4.0	50
56	A 'universal' B3LYP-based method for gas-phase molecular properties: bond dissociation enthalpy, ionization potential, electron and proton affinity and gas-phase acidity. Molecular Physics, 2005, 103, 815-823.	1.7	69
57	Theoretical and Synthetic Investigations of Carbodiimide Insertions into Al–CH3 and Al–N(CH3)2 Bonds. Inorganic Chemistry, 2005, 44, 1983-1991.	4.0	96