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	Catalytic Intermolecular Direct Arylation of Perfluorobenzenes. Journal of the American Chemical Society, 2006, 128, 8754-8756.	13.7	801
2	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
3	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
4	Simulation-Based Approaches for Determining Membrane Permeability of Small Compounds. Journal of Chemical Information and Modeling, 2016, 56, 721-733.	5.4	174
5	Ion selectivity in channels and transporters. Journal of General Physiology, 2011, 137, 415-426.	1.9	142
6	Molecular simulation of nonfacilitated membrane permeation. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1672-1687.	2.6	114
7	Theoretical and Synthetic Investigations of Carbodiimide Insertions into Alâ˜’CH3and Alâ˜’N(CH3)2Bonds. Inorganic Chemistry, 2005, 44, 1983-1991.	4.0	96
8	Why Can Hydrogen Sulfide Permeate Cell Membranes?. Journal of the American Chemical Society, 2014, 136, 15111-15113.	13.7	90
9	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
10	A â€˜universalâ€™ 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
11	Range-Separated DFT Functionals are Necessary to Model Thio-Michael Additions. Journal of Chemical Theory and Computation, 2013, 9, 4860-4865.	5.3	67
12	Modeling covalent-modifier drugs. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2017, 1865, 1664-1675.	2.3	67
13	Polarisable force fields: what do they add in biomolecular simulations?. Current Opinion in Structural Biology, 2020, 61, 182-190.	5.7	63
14	Ring-opening hydroarylation of monosubstituted cyclopropanes enabled by hexafluoroisopropanol. Chemical Science, 2018, 9, 6411-6416.	7.4	62
15	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
16	The CHARMMâ€“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
17	Simulating proteinâ€“ligand binding with neural network potentials. Chemical Science, 2020, 11, 2362-2368.	7.4	51
18	Synthesis and Thermolysis of Aluminum Amidinates:Â A Ligand-Exchange Route for New Mixed-Ligand Systems. Inorganic Chemistry, 2006, 45, 2276-2281.	4.0	50

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19	How Reactive are Druggable Cysteines in Protein Kinases?. Journal of Chemical Information and Modeling, 2018, 58, 1935-1946.	5.4	44
20	Unlocking the Friedel-Crafts arylation of primary aliphatic alcohols and epoxides driven by hexafluoroisopropanol. CheM, 2021, 7, 3425-3441.	11.7	44
21	DFT Study of the Isomerization and Spectroscopic/Structural Properties of Ruthenacyclobutane Intermediates Relevant to Olefin Metathesis. Organometallics, 2008, 27, 6043-6045.	2.3	42
22	Generalized Langevin Methods for Calculating Transmembrane Diffusivity. Journal of Chemical Theory and Computation, 2016, 12, 5609-5619.	5.3	42
23	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
24	Amidolithium and Amidoaluminum Catalyzed Synthesis of Substituted Guanidines: An Interplay of DFT Modeling and Experiment. Inorganic Chemistry, 2008, 47, 9660-9668.	4.0	39
25	Counteranion Effects on the Zirconocene Polymerization Catalyst Olefin Complex from QM/MM Molecular Dynamics Simulations. Organometallics, 2011, 30, 2071-2074.	2.3	37
26	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
27	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
28	Solvation of Hydrogen Sulfide in Liquid Water and at the Waterâ€“Vapor Interface Using a Polarizable Force Field. Journal of Physical Chemistry B, 2014, 118, 1373-1380.	2.6	31
29	Quantum Chemical Methods for Modeling Covalent Modification of Biological Thiols. Journal of Computational Chemistry, 2020, 41, 427-438.	3.3	31
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	Folding free energy landscapes of Î²-sheets with non-polarizable and polarizable CHARMM force fields. Journal of Chemical Physics, 2018, 149, 072317.	3.0	28
32	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
33	The tipping point of the inert pair effect: experimental and computational comparison of In(<scp>i</scp>) and Sn(<scp>ii</scp>) bis(imino)pyridine complexes. Dalton Transactions, 2014, 43, 690-697.	3.3	24
34	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
35	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
36	Mechanism of Olefin Hydrogenation Catalyzed by RuHCl(L)(PR₃)₂ Complexes (L) Tj ETQq0 0 0 rgBT /Overlock	2.3	22

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37	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
38	A Computational Experiment of the Endo versus Exo Preference in a Dielsâ€“Alder Reaction. Journal of Chemical Education, 2009, 86, 199.	2.3	22
39	Atom efficient cyclotrimerization of dimethylcyanamide catalyzed by aluminium amide: a combined experimental and theoretical investigation. Chemical Communications, 2008, , 3645.	4.1	21
40	A Drude Polarizable Model for Liquid Hydrogen Sulfide. Journal of Physical Chemistry B, 2013, 117, 5222-5229.	2.6	20
41	Automated computational screening of the thiol reactivity of substituted alkenes. Journal of Computer-Aided Molecular Design, 2015, 29, 725-735.	2.9	19
42	The hydration structure of methylthiolate from QM/MM molecular dynamics. Journal of Chemical Physics, 2018, 149, 045103.	3.0	18
43	Polarizable Force Field with a Ïƒ-Hole for Liquid and Aqueous Bromomethane. Journal of Physical Chemistry B, 2015, 119, 13422-13432.	2.6	17
44	Reaction Dynamics of Î²-Hydrogen Transfer in the Zirconocene Olefin Polymerization Catalyst: A DFT Path Sampling Study. Organometallics, 2008, 27, 6405-6407.	2.3	16
45	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
46	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
47	Mechanisms of Alkyl and Aryl Thiol Addition to N-Methylmaleimide. Journal of Organic Chemistry, 2018, 83, 11674-11685.	3.2	14
48	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
49	Modeling the Binding and Conformational Energetics of a Targeted Covalent Inhibitor to Brutonâ€™s Tyrosine Kinase. Journal of Chemical Information and Modeling, 2021, 61, 5234-5242.	5.4	12
50	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
51	An explicit-solvent conformation search method using open software. PeerJ, 2016, 4, e2088.	2.0	6
52	The hydration structure of carbon monoxide byab initiomethods. Journal of Chemical Physics, 2017, 146, 034503.	3.0	5
53	C(sp³)â€“C(sp³) Coupling with a Pd(II) Complex Bearing a Structurally Responsive Ligand. Organometallics, 2019, 38, 1677-1681.	2.3	4
54	An efficient and accurate model for water with an improved non-bonded potential. Journal of Chemical Physics, 2020, 153, 134105.	3.0	3

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55	Measuring and predicting warhead and residue reactivity. Annual Reports in Medicinal Chemistry, 2021, 56, 203-227.	0.9	2
56	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
57	Importance of Secondary Interactions in Twisted Doubly Hydrogen Bonded Complexes. Organic Letters, 2012, 14, 5772-5775.	4.6	1