

# Christopher N Rowley

## List of Publications by Year in descending order

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57  
papers

3,300  
citations

196777  
29  
h-index

162838  
57  
g-index

94  
all docs

94  
docs citations

94  
times ranked

4832  
citing authors

#	ARTICLE	IF	CITATIONS
1	Interaction between Antimicrobial Peptide Magainin 2 and Nonlipid Components in the Bacterial Outer Envelope. <i>Journal of Physical Chemistry B</i> , 2022, 126, 5473-5480.	1.2	2
2	Measuring and predicting warhead and residue reactivity. <i>Annual Reports in Medicinal Chemistry</i> , 2021, 56, 203-227.	0.5	2
3	Modeling the Binding and Conformational Energetics of a Targeted Covalent Inhibitor to Bruton's Tyrosine Kinase. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 5234-5242.	2.5	12
4	Unlocking the Friedel-Crafts arylation of primary aliphatic alcohols and epoxides driven by hexafluoroisopropanol. <i>CheM</i> , 2021, 7, 3425-3441.	5.8	44
5	Quantum Chemical Methods for Modeling Covalent Modification of Biological Thiols. <i>Journal of Computational Chemistry</i> , 2020, 41, 427-438.	1.5	31
6	Benchmarking Force Field and the ANI Neural Network Potentials for the Torsional Potential Energy Surface of Biaryl Drug Fragments. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 6258-6268.	2.5	15
7	Flexible Fitting of Small Molecules into Electron Microscopy Maps Using Molecular Dynamics Simulations with Neural Network Potentials. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 2591-2604.	2.5	24
8	Polarisable force fields: what do they add in biomolecular simulations?. <i>Current Opinion in Structural Biology</i> , 2020, 61, 182-190.	2.6	63
9	Simulating protein-ligand binding with neural network potentials. <i>Chemical Science</i> , 2020, 11, 2362-2368.	3.7	51
10	An efficient and accurate model for water with an improved non-bonded potential. <i>Journal of Chemical Physics</i> , 2020, 153, 134105.	1.2	3
11	C(sp <sup>3</sup> )-C(sp <sup>3</sup> ) Coupling with a Pd(II) Complex Bearing a Structurally Responsive Ligand. <i>Organometallics</i> , 2019, 38, 1677-1681.	1.1	4
12	Mechanisms of Alkyl and Aryl Thiol Addition to N-Methylmaleimide. <i>Journal of Organic Chemistry</i> , 2018, 83, 11674-11685.	1.7	14
13	Ring-opening hydroarylation of monosubstituted cyclopropanes enabled by hexafluoroisopropanol. <i>Chemical Science</i> , 2018, 9, 6411-6416.	3.7	62
14	The hydration structure of methylthiolate from QM/MM molecular dynamics. <i>Journal of Chemical Physics</i> , 2018, 149, 045103.	1.2	18
15	How Reactive are Druggable Cysteines in Protein Kinases?. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 1935-1946.	2.5	44
16	Evaluating the London Dispersion Coefficients of Protein Force Fields Using the Exchange-Hole Dipole Moment Model. <i>Journal of Physical Chemistry B</i> , 2018, 122, 6690-6701.	1.2	32
17	Folding free energy landscapes of $\beta$ -sheets with non-polarizable and polarizable CHARMM force fields. <i>Journal of Chemical Physics</i> , 2018, 149, 072317.	1.2	28
18	Simulations of lipid bilayers using the CHARMM36 force field with the TIP3P-FB and TIP4P-FB water models. <i>PeerJ</i> , 2018, 6, e5472.	0.9	23

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19	Modeling covalent-modifier drugs. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2017, 1865, 1664-1675.	1.1	67
20	Evaluating Force-Field London Dispersion Coefficients Using the Exchange-Hole Dipole Moment Model. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 6146-6157.	2.3	40
21	The hydration structure of carbon monoxide by ab initio methods. <i>Journal of Chemical Physics</i> , 2017, 146, 034503.	1.2	5
22	An explicit-solvent conformation search method using open software. <i>PeerJ</i> , 2016, 4, e2088.	0.9	6
23	Simulation-Based Approaches for Determining Membrane Permeability of Small Compounds. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 721-733.	2.5	174
24	Evaluation of Methods for the Calculation of the $pK_a$ of Cysteine Residues in Proteins. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4662-4673.	2.3	88
25	Generalized Langevin Methods for Calculating Transmembrane Diffusivity. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 5609-5619.	2.3	42
26	Molecular simulation of nonfacilitated membrane permeation. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2016, 1858, 1672-1687.	1.4	114
27	Polarizable Force Field with a $\pi$ -Hole for Liquid and Aqueous Bromomethane. <i>Journal of Physical Chemistry B</i> , 2015, 119, 13422-13432.	1.2	17
28	Automated computational screening of the thiol reactivity of substituted alkenes. <i>Journal of Computer-Aided Molecular Design</i> , 2015, 29, 725-735.	1.3	19
29	The CHARMM-TURBOMOLE interface for efficient and accurate QM/MM molecular dynamics, free energies, and excited state properties. <i>Journal of Computational Chemistry</i> , 2014, 35, 2076-2086.	1.5	51
30	Combined Experimental and Computational Studies on the Physical and Chemical Properties of the Renewable Amide, 3-Acetamido-5-acetylfuran. <i>ChemPhysChem</i> , 2014, 15, 4087-4094.	1.0	28
31	Solvation of Hydrogen Sulfide in Liquid Water and at the Water-Vapor Interface Using a Polarizable Force Field. <i>Journal of Physical Chemistry B</i> , 2014, 118, 1373-1380.	1.2	31
32	Why Can Hydrogen Sulfide Permeate Cell Membranes?. <i>Journal of the American Chemical Society</i> , 2014, 136, 15111-15113.	6.6	90
33	The tipping point of the inert pair effect: experimental and computational comparison of $\text{In}(\text{imino})$ and $\text{Sn}(\text{imino})$ bis(imino)pyridine complexes. <i>Dalton Transactions</i> , 2014, 43, 690-697.	1.6	24
34	Benchmarking Quantum Chemical Methods for the Calculation of Molecular Dipole Moments and Polarizabilities. <i>Journal of Physical Chemistry A</i> , 2014, 118, 3678-3687.	1.1	205
35	Range-Separated DFT Functionals are Necessary to Model Thio-Michael Additions. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4860-4865.	2.3	67
36	A Drude Polarizable Model for Liquid Hydrogen Sulfide. <i>Journal of Physical Chemistry B</i> , 2013, 117, 5222-5229.	1.2	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.	0.6	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.	0.9	16
39	Importance of Secondary Interactions in Twisted Doubly Hydrogen Bonded Complexes. Organic Letters, 2012, 14, 5772-5775.	2.4	1
40	The Solvation Structure of Na <sup>+</sup> and K <sup>+</sup> in Liquid Water Determined from High Level <i>ab Initio</i> Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2012, 8, 3526-3535.	2.3	191
41	Counteranion Effects on the Zirconocene Polymerization Catalyst Olefin Complex from QM/MM Molecular Dynamics Simulations. Organometallics, 2011, 30, 2071-2074.	1.1	37
42	Ion selectivity in channels and transporters. Journal of General Physiology, 2011, 137, 415-426.	0.9	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.	1.2	6
44	A Computational Experiment of the Endo versus Exo Preference in a Diels-Alder Reaction. Journal of Chemical Education, 2009, 86, 199.	1.1	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.	6.6	56
46	Atom efficient cyclotrimerization of dimethylcyanamide catalyzed by aluminium amide: a combined experimental and theoretical investigation. Chemical Communications, 2008, , 3645.	2.2	21
47	Reaction Dynamics of $\beta$ -Hydrogen Transfer in the Zirconocene Olefin Polymerization Catalyst: A DFT Path Sampling Study. Organometallics, 2008, 27, 6405-6407.	1.1	16
48	Mechanism of Olefin Hydrogenation Catalyzed by RuHCl(L)(PR <sub>3</sub> ) <sub>2</sub> Complexes (L) Tj ETQq0,0 0 rgBTJ/Overlock	1.1	22
49	A Path Sampling Study of Ru-Hydride-Catalyzed H <sub>2</sub> Hydrogenation of Ethylene. Journal of the American Chemical Society, 2008, 130, 7218-7219.	6.6	22
50	Analysis of the Critical Step in Catalytic Carbodiimide Transformation: Proton Transfer from Amines, Phosphines, and Alkynes to Guanidates, Phosphoguanidates, and Propiolamidates with Li and Al Catalysts. Inorganic Chemistry, 2008, 47, 12024-12031.	1.9	27
51	DFT Study of the Isomerization and Spectroscopic/Structural Properties of Ruthenacyclobutane Intermediates Relevant to Olefin Metathesis. Organometallics, 2008, 27, 6043-6045.	1.1	42
52	Amidolithium and Amidoaluminum Catalyzed Synthesis of Substituted Guanidines: An Interplay of DFT Modeling and Experiment. Inorganic Chemistry, 2008, 47, 9660-9668.	1.9	39
53	Generation of initial trajectories for transition path sampling of chemical reactions with <i>ab initio</i> molecular dynamics. Journal of Chemical Physics, 2007, 126, 024110.	1.2	12
54	Catalytic Intermolecular Direct Arylation of Perfluorobenzenes. Journal of the American Chemical Society, 2006, 128, 8754-8756.	6.6	801

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55	Synthesis and Thermolysis of Aluminum Amidinates: A Ligand-Exchange Route for New Mixed-Ligand Systems. <i>Inorganic Chemistry</i> , 2006, 45, 2276-2281.	1.9	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. <i>Molecular Physics</i> , 2005, 103, 815-823.	0.8	69
57	Theoretical and Synthetic Investigations of Carbodiimide Insertions into Al~CH <sub>3</sub> and Al~N(CH <sub>3</sub> ) <sub>2</sub> Bonds. <i>Inorganic Chemistry</i> , 2005, 44, 1983-1991.	1.9	96