Christopher N Rowley

List of Publications by Citations

58 papers	2,674 citations	26 h-index	51 g-index
94 ext. papers	2,990 ext. citations	5.3 avg, IF	5.64 L-index

#	Paper	IF	Citations
58	Catalytic intermolecular direct arylation of perfluorobenzenes. *Journal of the American Chemical Society*, **2006**, 128, 8754-6	16.4	729
57	Benchmarking quantum chemical methods for the calculation of molecular dipole moments and polarizabilities. *Journal of Physical Chemistry A*, **2014**, 118, 3678-87	2.8	163
56	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, 3526-35	6.4	162
55	Ion selectivity in channels and transporters. *Journal of General Physiology*, **2011**, 137, 415-26	3.4	127
54	Simulation-Based Approaches for Determining Membrane Permeability of Small Compounds. *Journal of Chemical Information and Modeling*, **2016**, 56, 721-33	6.1	127
53	Theoretical and synthetic investigations of carbodiimide insertions into Al-CH3 and Al-N(CH3)2 bonds. *Inorganic Chemistry*, **2005**, 44, 1983-91	5.1	93
52	Molecular simulation of nonfacilitated membrane permeation. *Biochimica Et Biophysica Acta - Biomembranes*, **2016**, 1858, 1672-87	3.8	84
51	Why can hydrogen sulfide permeate cell membranes?. *Journal of the American Chemical Society*, **2014**, 136, 15111-3	16.4	70
50	Evaluation of Methods for the Calculation of the pKa of Cysteine Residues in Proteins. *Journal of Chemical Theory and Computation*, **2016**, 12, 4662-73	6.4	63
49	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	58
48	Solution conformation of C-linked antifreeze glycoprotein analogues and modulation of ice recrystallization. *Journal of the American Chemical Society*, **2009**, 131, 15745-53	16.4	53
47	Modeling covalent-modifier drugs. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2017**, 1865, 1664-1675	4	52
46	Synthesis and thermolysis of aluminum amidinates: a ligand-exchange route for new mixed-ligand systems. *Inorganic Chemistry*, **2006**, 45, 2276-81	5.1	50
45	Range-Separated DFT Functionals are Necessary to Model Thio-Michael Additions. *Journal of Chemical Theory and Computation*, **2013**, 9, 4860-5	6.4	49
44	Ring-opening hydroarylation of monosubstituted cyclopropanes enabled by hexafluoroisopropanol. *Chemical Science*, **2018**, 9, 6411-6416	9.4	44
43	DFT Study of the Isomerization and Spectroscopic/Structural Properties of Ruthenacyclobutane Intermediates Relevant to Olefin Metathesis. *Organometallics*, **2008**, 27, 6043-6045	3.8	42
42	The CHARMM-TURBOMOLE interface for efficient and accurate QM/MM molecular dynamics, free energies, and excited state properties. *Journal of Computational Chemistry*, **2014**, 35, 2076-86	3.5	40

41	Amidolithium and amidoaluminum catalyzed synthesis of substituted guanidines: an interplay of DFT modeling and experiment. *Inorganic Chemistry*, **2008**, 47, 9660-8	5.1	38
40	Generalized Langevin Methods for Calculating Transmembrane Diffusivity. *Journal of Chemical Theory and Computation*, **2016**, 12, 5609-5619	6.4	33
39	Polarisable force fields: what do they add in biomolecular simulations?. *Current Opinion in Structural Biology*, **2020**, 61, 182-190	8.1	31
38	Counteranion Effects on the Zirconocene Polymerization Catalyst Olefin Complex from QM/MM Molecular Dynamics Simulations. *Organometallics*, **2011**, 30, 2071-2074	3.8	30
37	Evaluating Force-Field London Dispersion Coefficients Using the Exchange-Hole Dipole Moment Model. *Journal of Chemical Theory and Computation*, **2017**, 13, 6146-6157	6.4	29
36	QM/MM molecular dynamics simulations of the hydration of Mg(II) and Zn(II) ions. *Canadian Journal of Chemistry*, **2013**, 91, 552-558	0.9	29
35	How Reactive are Druggable Cysteines in Protein Kinases?. *Journal of Chemical Information and Modeling*, **2018**, 58, 1935-1946	6.1	27
34	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, 1373-80	3.4	27
33	Simulating protein-ligand binding with neural network potentials. *Chemical Science*, **2020**, 11, 2362-2368	9.4	26
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, 12024-31	5.1	26
31	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	3.4	23
30	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	4.3	21
29	A path sampling study of Ru-hydride-catalyzed H2 hydrogenation of ethylene. *Journal of the American Chemical Society*, **2008**, 130, 7218-9	16.4	21
28	Folding free energy landscapes of -sheets with non-polarizable and polarizable CHARMM force fields. *Journal of Chemical Physics*, **2018**, 149, 072317	3.9	20
27	Atom efficient cyclotrimerization of dimethylcyanamide catalyzed by aluminium amide: a combined experimental and theoretical investigation. *Chemical Communications*, **2008**, 3645-7	5.8	20
26	Mechanism of Olefin Hydrogenation Catalyzed by RuHCl(L)(PR3)2 Complexes (L = CO, PR3): A DFT Study. *Organometallics*, **2008**, 27, 1661-1663	3.8	19
25	Combined experimental and computational studies on the physical and chemical properties of the renewable amide, 3-acetamido-5-acetylfuran. *ChemPhysChem*, **2014**, 15, 4087-94	3.2	18
24	A Drude polarizable model for liquid hydrogen sulfide. *Journal of Physical Chemistry B*, **2013**, 117, 5222-9	3.4	18

23	A Computational Experiment of the Endo versus Exo Preference in a Diels–Alder Reaction. *Journal of Chemical Education*, **2009**, 86, 199	2.4	18
22	Simulations of lipid bilayers using the CHARMM36 force field with the TIP3P-FB and TIP4P-FB water models. *PeerJ*, **2018**, 6, e5472	3.1	18
21	Quantum Chemical Methods for Modeling Covalent Modification of Biological Thiols. *Journal of Computational Chemistry*, **2020**, 41, 427-438	3.5	18
20	Automated computational screening of the thiol reactivity of substituted alkenes. *Journal of Computer-Aided Molecular Design*, **2015**, 29, 725-35	4.2	17
19	Reaction Dynamics of β-Hydrogen Transfer in the Zirconocene Olefin Polymerization Catalyst: A DFT Path Sampling Study. *Organometallics*, **2008**, 27, 6405-6407	3.8	16
18	The hydration structure of methylthiolate from QM/MM molecular dynamics. *Journal of Chemical Physics*, **2018**, 149, 045103	3.9	15
17	Polarizable Force Field with a σ-Hole for Liquid and Aqueous Bromomethane. *Journal of Physical Chemistry B*, **2015**, 119, 13422-32	3.4	15
16	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, 451-63	3.4	13
15	Generation of initial trajectories for transition path sampling of chemical reactions with ab initio molecular dynamics. *Journal of Chemical Physics*, **2007**, 126, 024110	3.9	12
14	Unlocking the Friedel-Crafts arylation of primary aliphatic alcohols and epoxides driven by hexafluoroisopropanol. *CheM*, **2021**,	16.2	11
13	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	6.1	8
12	Computational design of ruthenium hydride olefin-hydrogenation catalysts containing hemilabile ligands,. *Canadian Journal of Chemistry*, **2009**, 87, 1030-1038	0.9	7
11	Mechanisms of Alkyl and Aryl Thiol Addition to N-Methylmaleimide. *Journal of Organic Chemistry*, **2018**, 83, 11674-11685	4.2	7
10	New shooting algorithms for transition path sampling: centering moves and varied-perturbation sizes for improved sampling. *Journal of Chemical Physics*, **2009**, 131, 234102	3.9	6
9	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	6.1	6
8	The hydration structure of carbon monoxide by ab initio methods. *Journal of Chemical Physics*, **2017**, 146, 034503	3.9	5
7	An explicit-solvent conformation search method using open software. *PeerJ*, **2016**, 4, e2088	3.1	5
6	Calculating the Full Free Energy Profile for Covalent Modification of a Druggable Cysteine in Bruton's Tyrosine Kinase		3

5	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	6.1	3
4	C(sp3)–C(sp3) Coupling with a Pd(II) Complex Bearing a Structurally Responsive Ligand. *Organometallics*, **2019**, 38, 1677-1681	3.8	2
3	Importance of secondary interactions in twisted doubly hydrogen bonded complexes. *Organic Letters*, **2012**, 14, 5772-5	6.2	1
2	An efficient and accurate model for water with an improved non-bonded potential. *Journal of Chemical Physics*, **2020**, 153, 134105	3.9	1
1	Measuring and predicting warhead and residue reactivity. *Annual Reports in Medicinal Chemistry*, **2021**, 56, 203-227	1.6	0