Benoit Roux

List of Publications by Citations

362 papers	31,811 citations	104 h-index	166 g-index
378 ext. papers	35,753 ext. citations	6.9 avg, IF	7.69 L-index

#	Paper	IF	Citations
362	The calculation of the potential of mean force using computer simulations. *Computer Physics Communications*, **1995**, 91, 275-282	4.2	1274
361	Finite representation of an infinite bulk system: Solvent boundary potential for computer simulations. *Journal of Chemical Physics*, **1994**, 100, 9050-9063	3.9	796
360	Energetics of ion conduction through the K+ channel. *Nature*, **2001**, 414, 73-7	50.4	659
359	Scalable molecular dynamics on CPU and GPU architectures with NAMD. *Journal of Chemical Physics* , **2020**, 153, 044130	3.9	483
358	Calculation of absolute protein-ligand binding free energy from computer simulations. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 6825-30	11.5	481
357	Continuum solvation model: Computation of electrostatic forces from numerical solutions to the Poisson-Boltzmann equation. *Computer Physics Communications*, **1998**, 111, 59-75	4.2	459
356	Control of ion selectivity in potassium channels by electrostatic and dynamic properties of carbonyl ligands. *Nature*, **2004**, 431, 830-4	50.4	453
355	A polarizable model of water for molecular dynamics simulations of biomolecules. *Chemical Physics Letters*, **2006**, 418, 245-249	2.5	448
354	Computations of standard binding free energies with molecular dynamics simulations. *Journal of Physical Chemistry B*, **2009**, 113, 2234-46	3.4	415
353	An Integral Equation To Describe the Solvation of Polar Molecules in Liquid Water. *Journal of Physical Chemistry B*, **1997**, 101, 7821-7826	3.4	409
352	Molecular determinants of gating at the potassium-channel selectivity filter. *Nature Structural and Molecular Biology*, **2006**, 13, 311-8	17.6	355
351	Atomic Radii for Continuum Electrostatics Calculations Based on Molecular Dynamics Free Energy Simulations. *Journal of Physical Chemistry B*, **1997**, 101, 5239-5248	3.4	352
350	Simulating Monovalent and Divalent Ions in Aqueous Solution Using a Drude Polarizable Force Field. *Journal of Chemical Theory and Computation*, **2010**, 6, 774-786	6.4	336
349	Energetics of ion conduction through the gramicidin channel. *Proceedings of the National Academy of Sciences of the United States of America*, **2004**, 101, 117-22	11.5	335
348	Dynamic coupling between the SH2 and SH3 domains of c-Src and Hck underlies their inactivation by C-terminal tyrosine phosphorylation. *Cell*, **2001**, 105, 115-26	56.2	329
347	Theoretical and computational models of biological ion channels. *Quarterly Reviews of Biophysics*, **2004**, 37, 15-103	7	321
346	Absolute hydration free energy scale for alkali and halide ions established from simulations with a polarizable force field. *Journal of Physical Chemistry B*, **2006**, 110, 3308-22	3.4	320

345	Ion permeation and selectivity of OmpF porin: a theoretical study based on molecular dynamics, Brownian dynamics, and continuum electrodiffusion theory. *Journal of Molecular Biology*, **2002**, 322, 851-69	6.5	312
344	An Empirical Polarizable Force Field Based on the Classical Drude Oscillator Model: Development History and Recent Applications. *Chemical Reviews*, **2016**, 116, 4983-5013	68.1	299
343	Molecular dynamics of the KcsA K(+) channel in a bilayer membrane. *Biophysical Journal*, **2000**, 78, 2900-17	4.9	289
342	Molecular modeling and dynamics studies with explicit inclusion of electronic polarizability. Theory and applications. *Theoretical Chemistry Accounts*, **2009**, 124, 11-28	1.9	285
341	Absolute binding free energy calculations using molecular dynamics simulations with restraining potentials. *Biophysical Journal*, **2006**, 91, 2798-814	2.9	284
340	Force Field for Peptides and Proteins based on the Classical Drude Oscillator. *Journal of Chemical Theory and Computation*, **2013**, 9, 5430-5449	6.4	274
339	Finding transition pathways using the string method with swarms of trajectories. *Journal of Physical Chemistry B*, **2008**, 112, 3432-40	3.4	252
338	Molecular dynamics study of hydration in ethanol-water mixtures using a polarizable force field. *Journal of Physical Chemistry B*, **2005**, 109, 6705-13	3.4	246
337	Structure, energetics, and dynamics of lipid-protein interactions: A molecular dynamics study of the gramicidin A channel in a DMPC bilayer. *Proteins: Structure, Function and Bioinformatics*, **1996**, 24, 92-114	4.2	246
336	Activation pathway of Src kinase reveals intermediate states as targets for drug design. *Nature Communications*, **2014**, 5, 3397	17.4	244
335	Closing in on the resting state of the Shaker K(+) channel. *Neuron*, **2007**, 56, 124-40	13.9	243
334	Determination of Electrostatic Parameters for a Polarizable Force Field Based on the Classical Drude Oscillator. *Journal of Chemical Theory and Computation*, **2005**, 1, 153-68	6.4	237
333	Ions and counterions in a biological channel: a molecular dynamics simulation of OmpF porin from Escherichia coli in an explicit membrane with 1 M KCl aqueous salt solution. *Journal of Molecular Biology*, **2002**, 319, 1177-97	6.5	230
332	Molecular mechanism of H+ conduction in the single-file water chain of the gramicidin channel. *Biophysical Journal*, **2002**, 82, 2304-16	2.9	229
331	Calculation of Standard Binding Free Energies: Aromatic Molecules in the T4 Lysozyme L99A Mutant. *Journal of Chemical Theory and Computation*, **2006**, 2, 1255-73	6.4	228
330	Structural basis for the coupling between activation and inactivation gates in K(+) channels. *Nature*, **2010**, 466, 272-5	50.4	227
329	Gating charge displacement in voltage-gated ion channels involves limited transmembrane movement. *Nature*, **2005**, 436, 852-6	50.4	226
328	Standard binding free energies from computer simulations: What is the best strategy?. *Journal of Chemical Theory and Computation*, **2013**, 9, 794-802	6.4	224

327	Simulation of Osmotic Pressure in Concentrated Aqueous Salt Solutions. *Journal of Physical Chemistry Letters*, **2010**, 1, 183-189	6.4	208
326	Molecular Dynamics Simulations of Ionic Liquids and Electrolytes Using Polarizable Force Fields. *Chemical Reviews*, **2019**, 119, 7940-7995	68.1	206
325	Molecular basis for the Born model of ion solvation. *The Journal of Physical Chemistry*, **1990**, 94, 4683-4688		204
324	Hydration of Amino Acid Side Chains: Nonpolar and Electrostatic Contributions Calculated from Staged Molecular Dynamics Free Energy Simulations with Explicit Water Molecules. *Journal of Physical Chemistry B*, **2004**, 108, 16567-16576	3.4	196
323	Molecular dynamics simulation of melittin in a dimyristoylphosphatidylcholine bilayer membrane. *Biophysical Journal*, **1998**, 75, 1603-18	2.9	196
322	A Grand Canonical Monte Carlo-Brownian dynamics algorithm for simulating ion channels. *Biophysical Journal*, **2000**, 79, 788-801	2.9	192
321	High-performance scalable molecular dynamics simulations of a polarizable force field based on classical Drude oscillators in NAMD. *Journal of Physical Chemistry Letters*, **2011**, 2, 87-92	6.4	191
320	Molecular driving forces determining potassium channel slow inactivation. *Nature Structural and Molecular Biology*, **2007**, 14, 1062-9	17.6	190
319	A microscopic view of ion conduction through the K+ channel. *Proceedings of the National Academy of Sciences of the United States of America*, **2003**, 100, 8644-8	11.5	189
318	Free energy profiles for H+ conduction along hydrogen-bonded chains of water molecules. *Biophysical Journal*, **1998**, 75, 33-40	2.9	182
317	Free Energy Perturbation Hamiltonian Replica-Exchange Molecular Dynamics (FEP/H-REMD) for Absolute Ligand Binding Free Energy Calculations. *Journal of Chemical Theory and Computation*, **2010**, 6, 2559-2565	6.4	180
316	Multidomain assembled states of Hck tyrosine kinase in solution. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 15757-62	11.5	177
315	A gate in the selectivity filter of potassium channels. *Structure*, **2005**, 13, 591-600	5.2	176
314	Structural mechanism of voltage-dependent gating in an isolated voltage-sensing domain. *Nature Structural and Molecular Biology*, **2014**, 21, 244-52	17.6	173
313	AUTOMATED FORCE FIELD PARAMETERIZATION FOR NON-POLARIZABLE AND POLARIZABLE ATOMIC MODELS BASED ON TARGET DATA. *Journal of Chemical Theory and Computation*, **2013**, 9,	6.4	172
312	Force field bias in protein folding simulations. *Biophysical Journal*, **2009**, 96, 3772-80	2.9	169
311	PBEQ-Solver for online visualization of electrostatic potential of biomolecules. *Nucleic Acids Research*, **2008**, 36, W270-5	20.1	163
310	Ion permeation through the alpha-hemolysin channel: theoretical studies based on Brownian dynamics and Poisson-Nernst-Plank electrodiffusion theory. *Biophysical Journal*, **2004**, 87, 2299-309	2.9	163

309	Atomic proximity between S4 segment and pore domain in Shaker potassium channels. *Neuron*, **2003**, 39, 467-81	13.9	163
308	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
307	Control of ion selectivity in LeuT: two Na+ binding sites with two different mechanisms. *Journal of Molecular Biology*, **2008**, 377, 804-18	6.5	160
306	Ion transport in a gramicidin-like channel: dynamics and mobility. *The Journal of Physical Chemistry*, **1991**, 95, 4856-4868		160
305	Importance of hydration and dynamics on the selectivity of the KcsA and NaK channels. *Journal of General Physiology*, **2007**, 129, 135-43	3.4	159
304	Ion channels, permeation, and electrostatics: insight into the function of KcsA. *Biochemistry*, **2000**, 39, 13295-306	3.2	158
303	Molecular dynamics - potential of mean force calculations as a tool for understanding ion permeation and selectivity in narrow channels. *Biophysical Chemistry*, **2006**, 124, 251-67	3.5	155
302	Solvation of complex molecules in a polar liquid: An integral equation theory. *Journal of Chemical Physics*, **1996**, 104, 8678-8689	3.9	153
301	Ion conduction and selectivity in K(+) channels. *Annual Review of Biophysics and Biomolecular Structure*, **2005**, 34, 153-71		148
300	Two atomic constraints unambiguously position the S4 segment relative to S1 and S2 segments in the closed state of Shaker K channel. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 7904-9	11.5	145
299	Ion selectivity in potassium channels. *Biophysical Chemistry*, **2006**, 124, 279-91	3.5	144
298	Instantaneous ion configurations in the K+ ion channel selectivity filter revealed by 2D IR spectroscopy. *Science*, **2016**, 353, 1040-1044	33.3	142
297	An emerging consensus on voltage-dependent gating from computational modeling and molecular dynamics simulations. *Journal of General Physiology*, **2012**, 140, 587-94	3.4	141
296	The membrane potential and its representation by a constant electric field in computer simulations. *Biophysical Journal*, **2008**, 95, 4205-16	2.9	140
295	On the statistical equivalence of restrained-ensemble simulations with the maximum entropy method. *Journal of Chemical Physics*, **2013**, 138, 084107	3.9	139
294	Recovery from slow inactivation in K+ channels is controlled by water molecules. *Nature*, **2013**, 501, 121-4	40.4	138
293	Efficient determination of protein-protein standard binding free energies from first principles. *Journal of Chemical Theory and Computation*, **2013**, 9,	6.4	133
292	Polarizable empirical force field for aromatic compounds based on the classical drude oscillator. *Journal of Physical Chemistry B*, **2007**, 111, 2873-85	3.4	132

291	Molecular basis of proton blockage in aquaporins. *Structure*, **2004**, 12, 65-74	5.2	132
290	Simulations of anionic lipid membranes: development of interaction-specific ion parameters and validation using NMR data. *Journal of Physical Chemistry B*, **2013**, 117, 10183-92	3.4	130
289	Ion selectivity in channels and transporters. *Journal of General Physiology*, **2011**, 137, 415-26	3.4	127
288	On the importance of atomic fluctuations, protein flexibility, and solvent in ion permeation. *Journal of General Physiology*, **2004**, 124, 679-90	3.4	127
287	Explaining why Gleevec is a specific and potent inhibitor of Abl kinase. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 1664-9	11.5	126
286	Computations of Absolute Solvation Free Energies of Small Molecules Using Explicit and Implicit Solvent Model. *Journal of Chemical Theory and Computation*, **2009**, 5, 919-30	6.4	125
285	Polarizable empirical force field for the primary and secondary alcohol series based on the classical Drude model. *Journal of Chemical Theory and Computation*, **2007**, 3, 1927-1946	6.4	124
284	Computational studies of the gramicidin channel. *Accounts of Chemical Research*, **2002**, 35, 366-75	24.3	124
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282	Atomic Level Anisotropy in the Electrostatic Modeling of Lone Pairs for a Polarizable Force Field Based on the Classical Drude Oscillator. *Journal of Chemical Theory and Computation*, **2006**, 2, 1587-97	6.4	123
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280	Dynamics of the Kv1.2 voltage-gated K+ channel in a membrane environment. *Biophysical Journal*, **2007**, 93, 3070-82	2.9	122
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277	CHARMM-GUI 10 years for biomolecular modeling and simulation. *Journal of Computational Chemistry*, **2017**, 38, 1114-1124	3.5	119
276	Constant electric field simulations of the membrane potential illustrated with simple systems. *Biochimica Et Biophysica Acta - Biomembranes*, **2012**, 1818, 294-302	3.8	119
275	Computational studies of membrane channels. *Structure*, **2004**, 12, 1343-51	5.2	119
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270	Statistical mechanical equilibrium theory of selective ion channels. *Biophysical Journal*, **1999**, 77, 139-53	2.9	116
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268	The Theory of Ultra-Coarse-Graining. 1. General Principles. *Journal of Chemical Theory and Computation*, **2013**, 9, 2466-80	6.4	114
267	Solvation Free Energy of Polar and Nonpolar Molecules in Water: An Extended Interaction Site Integral Equation Theory in Three Dimensions. *Journal of Physical Chemistry B*, **2000**, 104, 796-805	3.4	114
266	Understanding the dielectric properties of liquid amides from a polarizable force field. *Journal of Physical Chemistry B*, **2008**, 112, 3509-21	3.4	113
265	Free energy landscape of A-DNA to B-DNA conversion in aqueous solution. *Journal of the American Chemical Society*, **2005**, 127, 6866-76	16.4	113
264	Building Markov state models along pathways to determine free energies and rates of transitions. *Journal of Chemical Physics*, **2008**, 129, 064107	3.9	112
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235	Parametrization, molecular dynamics simulation, and calculation of electron spin resonance spectra of a nitroxide spin label on a polyalanine alpha-helix. *Journal of Physical Chemistry B*, **2008**, 112, 5755-67	3.4	84
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233	The ionization state and the conformation of Glu-71 in the KcsA K(+) channel. *Biophysical Journal*, **2002**, 82, 772-80	2.9	82
232	On the origin of the electrostatic potential difference at a liquid-vacuum interface. *Journal of Chemical Physics*, **2008**, 129, 234706	3.9	81
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230	Imaging the electrostatic potential of transmembrane channels: atomic probe microscopy of OmpF porin. *Biophysical Journal*, **2002**, 82, 1667-76	2.9	79
229	In search of a consensus model of the resting state of a voltage-sensing domain. *Neuron*, **2011**, 72, 713-20	8.9	78
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215	Molecular dynamics simulations of the influenza hemagglutinin fusion peptide in micelles and bilayers: conformational analysis of peptide and lipids. *Journal of Molecular Biology*, **2005**, 354, 1129-41	6.5	67
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199	Electrostatics of the intracellular vestibule of K+ channels. *Journal of Molecular Biology*, **2005**, 354, 272-88	3.5	57
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192	CHARMM-GUI Ligand Binder for absolute binding free energy calculations and its application. *Journal of Chemical Information and Modeling*, **2013**, 53, 267-77	6.1	51
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