Alexander D Mackerell

List of Publications by Citations

417 papers	51,479 citations	90 h-index	221 g-index
472 ext. papers	60,775 ext. citations	6 avg, IF	7.96 L-index

#	Paper	IF	Citations
417	CHARMM: the biomolecular simulation program. *Journal of Computational Chemistry*, **2009**, 30, 1545-614	3.5	5515
416	CHARMM general force field: A force field for drug-like molecules compatible with the CHARMM all-atom additive biological force fields. *Journal of Computational Chemistry*, **2010**, 31, 671-90	3.5	2953
415	Extending the treatment of backbone energetics in protein force fields: limitations of gas-phase quantum mechanics in reproducing protein conformational distributions in molecular dynamics simulations. *Journal of Computational Chemistry*, **2004**, 25, 1400-15	3.5	2792
414	Update of the CHARMM all-atom additive force field for lipids: validation on six lipid types. *Journal of Physical Chemistry B*, **2010**, 114, 7830-43	3.4	2654
413	Optimization of the additive CHARMM all-atom protein force field targeting improved sampling of the backbone □□ and side-chain (□1) and (□2) dihedral angles. *Journal of Chemical Theory and Computation*, **2012**, 8, 3257-3273	6.4	2511
412	CHARMM36m: an improved force field for folded and intrinsically disordered proteins. *Nature Methods*, **2017**, 14, 71-73	21.6	1819
411	CHARMM36 all-atom additive protein force field: validation based on comparison to NMR data. *Journal of Computational Chemistry*, **2013**, 34, 2135-45	3.5	1487
410	All-atom empirical force field for nucleic acids: I. Parameter optimization based on small molecule and condensed phase macromolecular target data. *Journal of Computational Chemistry*, **2000**, 21, 86-104	3.5	1308
409	CHARMM-GUI Input Generator for NAMD, GROMACS, AMBER, OpenMM, and CHARMM/OpenMM Simulations Using the CHARMM36 Additive Force Field. *Journal of Chemical Theory and Computation*, **2016**, 12, 405-13	6.4	1303
408	Empirical force fields for biological macromolecules: overview and issues. *Journal of Computational Chemistry*, **2004**, 25, 1584-604	3.5	1006
407	Automation of the CHARMM General Force Field (CGenFF) I: bond perception and atom typing. *Journal of Chemical Information and Modeling*, **2012**, 52, 3144-54	6.1	908
406	Automation of the CHARMM General Force Field (CGenFF) II: assignment of bonded parameters and partial atomic charges. *Journal of Chemical Information and Modeling*, **2012**, 52, 3155-68	6.1	852
405	Development and current status of the CHARMM force field for nucleic acids. *Biopolymers*, **2000**, 56, 257-65	2.2	795
404	Improved treatment of the protein backbone in empirical force fields. *Journal of the American Chemical Society*, **2004**, 126, 698-9	16.4	773
403	An Improved Empirical Potential Energy Function for Molecular Simulations of Phospholipids. *Journal of Physical Chemistry B*, **2000**, 104, 7510-7515	3.4	680
402	All-atom empirical force field for nucleic acids: II. Application to molecular dynamics simulations of DNA and RNA in solution. *Journal of Computational Chemistry*, **2000**, 21, 105-120	3.5	648
401	An all-atom empirical energy function for the simulation of nucleic acids. *Journal of the American Chemical Society*, **1995**, 117, 11946-11975	16.4	633

400	A simple polarizable model of water based on classical Drude oscillators. *Journal of Chemical Physics*, **2003**, 119, 5185-5197	3.9	584
399	CHARMM Additive All-Atom Force Field for Glycosidic Linkages between Hexopyranoses. *Journal of Chemical Theory and Computation*, **2009**, 5, 2353-2370	6.4	473
398	A polarizable model of water for molecular dynamics simulations of biomolecules. *Chemical Physics Letters*, **2006**, 418, 245-249	2.5	448
397	Extension of the CHARMM General Force Field to sulfonyl-containing compounds and its utility in biomolecular simulations. *Journal of Computational Chemistry*, **2012**, 33, 2451-68	3.5	447
396	Additive empirical force field for hexopyranose monosaccharides. *Journal of Computational Chemistry*, **2008**, 29, 2543-64	3.5	421
395	CHARMM additive all-atom force field for carbohydrate derivatives and its utility in polysaccharide and carbohydrate-protein modeling. *Journal of Chemical Theory and Computation*, **2011**, 7, 3162-3180	6.4	403
394	Polyunsaturated fatty acids in lipid bilayers: intrinsic and environmental contributions to their unique physical properties. *Journal of the American Chemical Society*, **2002**, 124, 318-26	16.4	386
393	CHARMM fluctuating charge force field for proteins: II protein/solvent properties from molecular dynamics simulations using a nonadditive electrostatic model. *Journal of Computational Chemistry*, **2004**, 25, 1504-14	3.5	371
392	Optimization of the CHARMM additive force field for DNA: Improved treatment of the BI/BII conformational equilibrium. *Journal of Chemical Theory and Computation*, **2012**, 8, 348-362	6.4	348
391	Molecular dynamics studies of polyethylene oxide and polyethylene glycol: hydrodynamic radius and shape anisotropy. *Biophysical Journal*, **2008**, 95, 1590-9	2.9	347
390	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
389	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
388	Molecular modeling and dynamics studies with explicit inclusion of electronic polarizability. Theory and applications. *Theoretical Chemistry Accounts*, **2009**, 124, 11-28	1.9	285
387	An ab initio study on the torsional surface of alkanes and its effect on molecular simulations of alkanes and a DPPC bilayer. *Journal of Physical Chemistry B*, **2005**, 109, 5300-11	3.4	279
386	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
385	Importance of the CMAP correction to the CHARMM22 protein force field: dynamics of hen lysozyme. *Biophysical Journal*, **2006**, 90, L36-8	2.9	263
384	Impact of 2Phydroxyl sampling on the conformational properties of RNA: update of the CHARMM all-atom additive force field for RNA. *Journal of Computational Chemistry*, **2011**, 32, 1929-43	3.5	249
383	Development of the CHARMM Force Field for Lipids. *Journal of Physical Chemistry Letters*, **2011**, 2, 1526-1532	6.4	240

382	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
381	Molecular Dynamics Simulation Analysis of a Sodium Dodecyl Sulfate Micelle in Aqueous Solution: Decreased Fluidity of the Micelle Hydrocarbon Interior. *The Journal of Physical Chemistry*, **1995**, 99, 1846-1855		237
380	A small-molecule inhibitor of BCL6 kills DLBCL cells in vitro and in vivo. *Cancer Cell*, **2010**, 17, 400-11	24.3	230
379	Decoding the signaling of a GPCR heteromeric complex reveals a unifying mechanism of action of antipsychotic drugs. *Cell*, **2011**, 147, 1011-23	56.2	226
378	The structure of aqueous guanidinium chloride solutions. *Journal of the American Chemical Society*, **2004**, 126, 11462-70	16.4	214
377	Additive and Classical Drude Polarizable Force Fields for Linear and Cyclic Ethers. *Journal of Chemical Theory and Computation*, **2007**, 3, 1120-33	6.4	210
376	Molecular Dynamics Simulations of Ionic Liquids and Electrolytes Using Polarizable Force Fields. *Chemical Reviews*, **2019**, 119, 7940-7995	68.1	206
375	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
374	Force Field Influence on the Observation of Helical Protein Structures in Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2003**, 107, 2831-2836	3.4	186
373	Development of an empirical force field for silica. Application to the quartz-water interface. *Journal of Physical Chemistry B*, **2006**, 110, 2782-92	3.4	181
372	Polarizable empirical force field for alkanes based on the classical Drude oscillator model. *Journal of Physical Chemistry B*, **2005**, 109, 18988-99	3.4	173
371	Combined ab initio/empirical approach for optimization of Lennard-Jones parameters. *Journal of Computational Chemistry*, **1998**, 19, 334-348	3.5	164
370	Computational fragment-based binding site identification by ligand competitive saturation. *PLoS Computational Biology*, **2009**, 5, e1000435	5	161
369	Computer-Aided Drug Design Methods. *Methods in Molecular Biology*, **2017**, 1520, 85-106	1.4	160
368	An Empirical Potential Energy Function for Phospholipids: Criteria for Parameter Optimization and Applications **1996**, 31-81		154
367	CHARMM additive and polarizable force fields for biophysics and computer-aided drug design. *Biochimica Et Biophysica Acta - General Subjects*, **2015**, 1850, 861-871	4	150
366	Molecular-level organization of saturated and polyunsaturated fatty acids in a phosphatidylcholine bilayer containing cholesterol. *Biochemistry*, **2004**, 43, 15318-28	3.2	150
365	Recent advances in ligand-based drug design: relevance and utility of the conformationally sampled pharmacophore approach. *Current Computer-Aided Drug Design*, **2011**, 7, 10-22	1.4	149

364	Recent Developments and Applications of the CHARMM force fields. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 167-185	7.9	139
363	A molecular mechanics force field for NAD+ NADH, and the pyrophosphate groups of nucleotides. *Journal of Computational Chemistry*, **1997**, 18, 221-239	3.5	139
362	Free energy and structural pathways of base flipping in a DNA GCGC containing sequence. *Journal of Molecular Biology*, **2002**, 319, 141-60	6.5	139
361	CHARMM all-atom additive force field for sphingomyelin: elucidation of hydrogen bonding and of positive curvature. *Biophysical Journal*, **2014**, 107, 134-45	2.9	138
360	Molecular dynamics simulations of nucleic acid-protein complexes. *Current Opinion in Structural Biology*, **2008**, 18, 194-9	8.1	135
359	Rational design of human DNA ligase inhibitors that target cellular DNA replication and repair. *Cancer Research*, **2008**, 68, 3169-77	10.1	132
358	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
357	Comparison of protein force fields for molecular dynamics simulations. *Methods in Molecular Biology*, **2008**, 443, 63-88	1.4	132
356	CHARMM additive all-atom force field for glycosidic linkages in carbohydrates involving furanoses. *Journal of Physical Chemistry B*, **2010**, 114, 12981-94	3.4	129
355	Consideration of molecular weight during compound selection in virtual target-based database screening. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 267-72		128
354	A hybrid mechanism of action for BCL6 in B cells defined by formation of functionally distinct complexes at enhancers and promoters. *Cell Reports*, **2013**, 4, 578-88	10.6	127
353	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
352	CHARMM Additive All-Atom Force Field for Acyclic Polyalcohols, Acyclic Carbohydrates and Inositol. *Journal of Chemical Theory and Computation*, **2009**, 5, 1315-1327	6.4	123
351	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
350	A polarizable force field of dipalmitoylphosphatidylcholine based on the classical Drude model for molecular dynamics simulations of lipids. *Journal of Physical Chemistry B*, **2013**, 117, 9142-60	3.4	122
349	CHARMM-GUI 10 years for biomolecular modeling and simulation. *Journal of Computational Chemistry*, **2017**, 38, 1114-1124	3.5	119
348	Glycan Reader: automated sugar identification and simulation preparation for carbohydrates and glycoproteins. *Journal of Computational Chemistry*, **2011**, 32, 3135-41	3.5	118
347	Protein-facilitated base flipping in DNA by cytosine-5-methyltransferase. *Proceedings of the National Academy of Sciences of the United States of America*, **2003**, 100, 68-73	11.5	117

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345	All-atom polarizable force field for DNA based on the classical Drude oscillator model. *Journal of Computational Chemistry*, **2014**, 35, 1219-39	3.5	115
344	Intrinsic conformational properties of deoxyribonucleosides: implicated role for cytosine in the equilibrium among the A, B, and Z forms of DNA. *Biophysical Journal*, **1999**, 76, 3206-18	2.9	115
343	Understanding the dielectric properties of liquid amides from a polarizable force field. *Journal of Physical Chemistry B*, **2008**, 112, 3509-21	3.4	113
342	Recent Advances in Polarizable Force Fields for Macromolecules: Microsecond Simulations of Proteins Using the Classical Drude Oscillator Model. *Journal of Physical Chemistry Letters*, **2014**, 5, 3144-3150	6.4	111
341	Current status of protein force fields for molecular dynamics simulations. *Methods in Molecular Biology*, **2015**, 1215, 47-71	1.4	108
340	CHARMM additive all-atom force field for aldopentofuranoses, methyl-aldopentofuranosides, and fructofuranose. *Journal of Physical Chemistry B*, **2009**, 113, 12466-76	3.4	107
339	Inclusion of many-body effects in the additive CHARMM protein CMAP potential results in enhanced cooperativity of α-helix and β-hairpin formation. *Biophysical Journal*, **2012**, 103, 1045-51	2.9	105
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337	Development of a polarizable intermolecular potential function (PIPF) for liquid amides and alkanes. *Journal of Chemical Theory and Computation*, **2007**, 3, 1878-1889	6.4	102
336	Identification of novel extracellular signal-regulated kinase docking domain inhibitors. *Journal of Medicinal Chemistry*, **2005**, 48, 4586-95	8.3	98
335	Intrinsic conformational energetics associated with the glycosyl torsion in DNA: a quantum mechanical study. *Biophysical Journal*, **2002**, 82, 1554-69	2.9	98
334	Force field development and simulations of intrinsically disordered proteins. *Current Opinion in Structural Biology*, **2018**, 48, 40-48	8.1	98
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332	Parametrization of halogen bonds in the CHARMM general force field: Improved treatment of ligand-protein interactions. *Bioorganic and Medicinal Chemistry*, **2016**, 24, 4812-4825	3.4	95
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330	Six-site polarizable model of water based on the classical Drude oscillator. *Journal of Chemical Physics*, **2013**, 138, 034508	3.9	92
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328	Rationally designed BCL6 inhibitors target activated B cell diffuse large B cell lymphoma. *Journal of Clinical Investigation*, **2016**, 126, 3351-62	15.9	92
327	Many-body polarization effects and the membrane dipole potential. *Journal of the American Chemical Society*, **2009**, 131, 2760-1	16.4	90
326	Automated conformational energy fitting for force-field development. *Journal of Molecular Modeling*, **2008**, 14, 667-79	2	90
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324	A small molecule agonist of EphA2 receptor tyrosine kinase inhibits tumor cell migration in vitro and prostate cancer metastasis in vivo. *PLoS ONE*, **2012**, 7, e42120	3.7	88
323	Simulation study of ion pairing in concentrated aqueous salt solutions with a polarizable force field. *Faraday Discussions*, **2013**, 160, 135-49; discussion 207-24	3.6	86
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319	Influence of Magnesium Ions on Duplex DNA Structural, Dynamic, and Solvation Properties. *Journal of Physical Chemistry B*, **1997**, 101, 646-650	3.4	82
318	Identification and characterization of small molecule inhibitors of the calcium-dependent S100B-p53 tumor suppressor interaction. *Journal of Medicinal Chemistry*, **2004**, 47, 5085-93	8.3	82
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316	Inhibition of TLR2 signaling by small molecule inhibitors targeting a pocket within the TLR2 TIR domain. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 5455-60	11.5	80
315	Inclusion of multiple fragment types in the site identification by ligand competitive saturation (SILCS) approach. *Journal of Chemical Information and Modeling*, **2013**, 53, 3384-98	6.1	79
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313	Computational identification of inhibitors of protein-protein interactions. *Current Topics in Medicinal Chemistry*, **2007**, 7, 63-82	3	77
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311	Is arginine charged in a membrane?. *Biophysical Journal*, **2008**, 94, L11-3	2.9	74

310	Computational approaches for investigating base flipping in oligonucleotides. *Chemical Reviews*, **2006**, 106, 489-505	68.1	73
309	Conformational Properties of the Deoxyribose and Ribose Moieties of Nucleic Acids: A Quantum Mechanical Study. *Journal of Physical Chemistry B*, **1998**, 102, 6669-6678	3.4	71
308	Structure, force, and energy of a double-stranded DNA oligonucleotide under tensile loads. *European Biophysics Journal*, **1999**, 28, 415-26	1.9	71
307	The novel BH3 α-helix mimetic JY-1-106 induces apoptosis in a subset of cancer cells (lung cancer, colon cancer and mesothelioma) by disrupting Bcl-xL and Mcl-1 protein-protein interactions with Bak. *Molecular Cancer*, **2013**, 12, 42	42.1	69
306	A piRNA-like small RNA interacts with and modulates p-ERM proteins in human somatic cells. *Nature Communications*, **2015**, 6, 7316	17.4	68
305	Competition among Li(+), Na(+), K(+), and Rb(+) monovalent ions for DNA in molecular dynamics simulations using the additive CHARMM36 and Drude polarizable force fields. *Journal of Physical Chemistry B*, **2015**, 119, 4428-40	3.4	66
304	Ab initio conformational analysis of nucleic acid components: intrinsic energetic contributions to nucleic acid structure and dynamics. *Biopolymers*, **2001**, 61, 61-76	2.2	65
303	Molecular simulations of dodecyl-β-maltoside micelles in water: influence of the headgroup conformation and force field parameters. *Journal of Physical Chemistry B*, **2011**, 115, 487-99	3.4	64
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300	Computational evaluation of protein-small molecule binding. *Current Opinion in Structural Biology*, **2009**, 19, 56-61	8.1	63
299	Balancing the interactions of ions, water, and DNA in the Drude polarizable force field. *Journal of Physical Chemistry B*, **2014**, 118, 6742-57	3.4	62
298	Polarizable empirical force field for nitrogen-containing heteroaromatic compounds based on the classical Drude oscillator. *Journal of Computational Chemistry*, **2009**, 30, 1821-38	3.5	62
297	Urea destabilizes RNA by forming stacking interactions and multiple hydrogen bonds with nucleic acid bases. *Journal of the American Chemical Society*, **2009**, 131, 17759-61	16.4	62
296	Induction of peptide bond dipoles drives cooperative helix formation in the (AAQAA)3 peptide. *Biophysical Journal*, **2014**, 107, 991-7	2.9	60
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294	Identification and validation of human DNA ligase inhibitors using computer-aided drug design. *Journal of Medicinal Chemistry*, **2008**, 51, 4553-62	8.3	60
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291	The BioFragment Database (BFDb): An open-data platform for computational chemistry analysis of noncovalent interactions. *Journal of Chemical Physics*, **2017**, 147, 161727	3.9	57
290	Novel LRRK2 GTP-binding inhibitors reduced degeneration in Parkinson's disease cell and mouse models. *Human Molecular Genetics*, **2014**, 23, 6212-22	5.6	57
289	Identification of non-phosphate-containing small molecular weight inhibitors of the tyrosine kinase p56 Lck SH2 domain via in silico screening against the pY + 3 binding site. *Journal of Medicinal Chemistry*, **2004**, 47, 3502-11	8.3	57
288	Molecular mechanics. *Current Pharmaceutical Design*, **2014**, 20, 3281-92	3.3	57
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286	Polarizable empirical force field for hexopyranose monosaccharides based on the classical Drude oscillator. *Journal of Physical Chemistry B*, **2015**, 119, 637-52	3.4	55
285	Contribution of the Phosphodiester Backbone and Glycosyl Linkage Intrinsic Torsional Energetics to DNA Structure and Dynamics. *Journal of Physical Chemistry B*, **1999**, 103, 10955-10964	3.4	54
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283	Small-molecule inhibitors of the ERK signaling pathway: Towards novel anticancer therapeutics. *ChemMedChem*, **2011**, 6, 38-48	3.7	53
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264	Polarizable Force Field for DNA Based on the Classical Drude Oscillator: II. Microsecond Molecular Dynamics Simulations of Duplex DNA. *Journal of Chemical Theory and Computation*, **2017**, 13, 2072-2085	6.4	46
263	Site-Identification by Ligand Competitive Saturation (SILCS) assisted pharmacophore modeling. *Journal of Computer-Aided Molecular Design*, **2014**, 28, 491-507	4.2	46
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