

# Alexander D Mackerell Jr

## List of Publications by Year in descending order

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55  
papers

13,882  
citations

117453

34  
h-index

161609

54  
g-index

56  
all docs

56  
docs citations

56  
times ranked

15210  
citing authors

#	ARTICLE	IF	CITATIONS
1	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. <i>Journal of Computational Chemistry</i> , 2004, 25, 1400-1415.	1.5	3,145
2	CHARMM36 all-atom additive protein force field: Validation based on comparison to NMR data. <i>Journal of Computational Chemistry</i> , 2013, 34, 2135-2145.	1.5	2,613
3	Empirical force fields for biological macromolecules: Overview and issues. <i>Journal of Computational Chemistry</i> , 2004, 25, 1584-1604.	1.5	1,134
4	Development and current status of the CHARMM force field for nucleic acids. <i>Biopolymers</i> , 2000, 56, 257-265.	1.2	923
5	All-atom empirical force field for nucleic acids: II. Application to molecular dynamics simulations of DNA and RNA in solution. <i>Journal of Computational Chemistry</i> , 2000, 21, 105-120.	1.5	701
6	Extension of the CHARMM general force field to sulfonyl-containing compounds and its utility in biomolecular simulations. <i>Journal of Computational Chemistry</i> , 2012, 33, 2451-2468.	1.5	659
7	A simple polarizable model of water based on classical Drude oscillators. <i>Journal of Chemical Physics</i> , 2003, 119, 5185-5197.	1.2	635
8	Additive empirical force field for hexopyranose monosaccharides. <i>Journal of Computational Chemistry</i> , 2008, 29, 2543-2564.	1.5	483
9	CHARMM fluctuating charge force field for proteins: II Protein/solvent properties from molecular dynamics simulations using a nonadditive electrostatic model. <i>Journal of Computational Chemistry</i> , 2004, 25, 1504-1514.	1.5	410
10	Molecular Dynamics Simulations of Ionic Liquids and Electrolytes Using Polarizable Force Fields. <i>Chemical Reviews</i> , 2019, 119, 7940-7995.	23.0	386
11	Impact of 2'-OH sampling on the conformational properties of RNA: Update of the CHARMM all-atom additive force field for RNA. <i>Journal of Computational Chemistry</i> , 2011, 32, 1929-1943.	1.5	341
12	The Structure of Aqueous Guanidinium Chloride Solutions. <i>Journal of the American Chemical Society</i> , 2004, 126, 11462-11470.	6.6	245
13	Computational Fragment-Based Binding Site Identification by Ligand Competitive Saturation. <i>PLoS Computational Biology</i> , 2009, 5, e1000435.	1.5	208
14	Combined ab initio/empirical approach for optimization of Lennard-Jones parameters. <i>Journal of Computational Chemistry</i> , 1998, 19, 334-348.	1.5	181
15	Recent developments and applications of the CHARMM force fields. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2012, 2, 167-185.	6.2	173
16	All-atom polarizable force field for DNA based on the classical drude oscillator model. <i>Journal of Computational Chemistry</i> , 2014, 35, 1219-1239.	1.5	136
17	Development of a Polarizable Intermolecular Potential Function (PIPF) for Liquid Amides and Alkanes. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1878-1889.	2.3	107
18	Six-site polarizable model of water based on the classical Drude oscillator. <i>Journal of Chemical Physics</i> , 2013, 138, 034508.	1.2	103

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19	Combined ab initio/empirical approach for optimization of Lennard-Jones parameters for polar-neutral compounds. <i>Journal of Computational Chemistry</i> , 2002, 23, 199-213.	1.5	100
20	CH/π interactions involving aromatic amino acids: Refinement of the CHARMM tryptophan force field. <i>Journal of Computational Chemistry</i> , 2005, 26, 1452-1463.	1.5	83
21	Molecular dynamics simulations using the drude polarizable force field on GPUs with OpenMM: Implementation, validation, and benchmarks. <i>Journal of Computational Chemistry</i> , 2018, 39, 1682-1689.	1.5	77
22	Ab initio conformational analysis of nucleic acid components: Intrinsic energetic contributions to nucleic acid structure and dynamics. <i>Biopolymers</i> , 2001, 61, 61-76.	1.2	70
23	Polarizable force field for RNA based on the classical drude oscillator. <i>Journal of Computational Chemistry</i> , 2018, 39, 2624-2646.	1.5	67
24	Polarizable empirical force field for nitrogen-containing heteroaromatic compounds based on the classical Drude oscillator. <i>Journal of Computational Chemistry</i> , 2009, 30, 1821-1838.	1.5	65
25	Additive CHARMM force field for naturally occurring modified ribonucleotides. <i>Journal of Computational Chemistry</i> , 2016, 37, 896-912.	1.5	63
26	Further Optimization and Validation of the Classical Drude Polarizable Protein Force Field. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3221-3239.	2.3	53
27	Polarizable Empirical Force Field for Acyclic Polyalcohols Based on the Classical Drude Oscillator. <i>Biopolymers</i> , 2013, 99, 724-738.	1.2	50
28	FFParam: Standalone package for CHARMM additive and Drude polarizable force field parametrization of small molecules. <i>Journal of Computational Chemistry</i> , 2020, 41, 958-970.	1.5	50
29	CHARMM force field parameters for simulation of reactive intermediates in native and thio-substituted ribozymes. <i>Journal of Computational Chemistry</i> , 2007, 28, 495-507.	1.5	49
30	Polarizable empirical force field for sulfur-containing compounds based on the classical Drude oscillator model. <i>Journal of Computational Chemistry</i> , 2010, 31, 2330-2341.	1.5	45
31	Polarizable Force Field for Molecular Ions Based on the Classical Drude Oscillator. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 993-1004.	2.5	45
32	Optimized Lennard-Jones Parameters for Druglike Small Molecules. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3121-3131.	2.3	44
33	Mapping the Drude polarizable force field onto a multipole and induced dipole model. <i>Journal of Chemical Physics</i> , 2017, 147, 161702.	1.2	42
34	Structural mechanism associated with domain opening in gain-of-function mutations in SHP2 phosphatase. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011, 79, 1573-1588.	1.5	37
35	Balancing target flexibility and target denaturation in computational fragment-based inhibitor discovery. <i>Journal of Computational Chemistry</i> , 2012, 33, 1880-1891.	1.5	36
36	Kirkwood-Buff analysis of aqueous N-methylacetamide and acetamide solutions modeled by the CHARMM additive and Drude polarizable force fields. <i>Journal of Chemical Physics</i> , 2013, 139, 084509.	1.2	31

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37	CHARMM Drude Polarizable Force Field for Glycosidic Linkages Involving Pyranoses and Furanoses. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3132-3143.	2.3	29
38	Improved Modeling of Cation- $\pi$ and Anion- $\pi$ Ring Interactions Using the Drude Polarizable Empirical Force Field for Proteins. <i>Journal of Computational Chemistry</i> , 2020, 41, 439-448.	1.5	27
39	Polarization Effects in Water-Mediated Selective Cation Transport across a Narrow Transmembrane Channel. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 1726-1741.	2.3	26
40	CHARMM-GUI Drude prepper for molecular dynamics simulation using the classical Drude polarizable force field. <i>Journal of Computational Chemistry</i> , 2022, 43, 359-375.	1.5	24
41	Improved Modeling of Halogenated Ligand-Protein Interactions Using the Drude Polarizable and CHARMM Additive Empirical Force Fields. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 215-228.	2.5	23
42	Toward Prediction of Electrostatic Parameters for Force Fields That Explicitly Treat Electronic Polarization. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2460-2469.	2.3	21
43	Drude Polarizable Force Field Parametrization of Carboxylate and <i>N</i> -Acetyl Amine Carbohydrate Derivatives. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4982-5000.	2.3	20
44	Rapid estimation of hydration thermodynamics of macromolecular regions. <i>Journal of Chemical Physics</i> , 2013, 139, 055105.	1.2	19
45	Impact of Ribosomal Modification on the Binding of the Antibiotic Telithromycin Using a Combined Grand Canonical Monte Carlo/Molecular Dynamics Simulation Approach. <i>PLoS Computational Biology</i> , 2013, 9, e1003113.	1.5	18
46	Harnessing Deep Learning for Optimization of Lennard-Jones Parameters for the Polarizable Classical Drude Oscillator Force Field. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2388-2407.	2.3	17
47	DIRECT: An automated method to identify and quantify conformational variations' application to $\beta$ -adrenergic GPCR. <i>Journal of Computational Chemistry</i> , 2016, 37, 416-425.	1.5	13
48	Deep Neural Network Model to Predict the Electrostatic Parameters in the Polarizable Classical Drude Oscillator Force Field. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 1711-1725.	2.3	13
49	Statistical mechanics of polarizable force fields based on classical Drude oscillators with dynamical propagation by the dual-thermostat extended Lagrangian. <i>Journal of Chemical Physics</i> , 2020, 153, 114108.	1.2	11
50	Hydrophobic residues in small ankyrin 1 participate in binding to obscurin. <i>Molecular Membrane Biology</i> , 2012, 29, 36-51.	2.0	7
51	DNA bending induced by carbocyclic sugar analogs constrained to the north conformation. <i>Biopolymers</i> , 2007, 85, 438-449.	1.2	5
52	(Ala) <sub>4</sub> -X-(Ala) <sub>4</sub> as a model system for the optimization of the $\phi$ <sub>1</sub> and $\phi$ <sub>2</sub> amino acid side-chain dihedral empirical force field parameters. <i>Journal of Computational Chemistry</i> , 2013, 34, 593-603.	1.5	5
53	Predicting Partition Coefficients of Neutral and Charged Solutes in the Mixed SLES-Fatty Acid Micellar System. <i>Journal of Physical Chemistry B</i> , 2020, 124, 1653-1664.	1.2	5
54	Insights into substrate recognition and specificity for IgG by Endoglycosidase S2. <i>PLoS Computational Biology</i> , 2021, 17, e1009103.	1.5	5

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55	Development of CHARMM Additive Potential Energy Parameters for $\hat{\pm}$ -Methyl Amino Acids. Journal of Physical Chemistry B, 2021, 125, 11687-11696.	1.2	0