Alexander D Mackerell Jr

List of Publications by Year
in descending order

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	Deep Neural Network Model to Predict the Electrostatic Parameters in the Polarizable Classical Drude Oscillator Force Field. Journal of Chemical Theory and Computation, 2022, 18, 1711-1725.	2.3	13
2	Harnessing Deep Learning for Optimization of Lennard-Jones Parameters for the Polarizable Classical Drude Oscillator Force Field. Journal of Chemical Theory and Computation, 2022, 18, 2388-2407.	2.3	17
3	<scp>CHARMMâ€GUI</scp> Drude prepper for molecular dynamics simulation using the classical Drude polarizable force field. Journal of Computational Chemistry, 2022, 43, 359-375.	1.5	24
4	Polarization Effects in Water-Mediated Selective Cation Transport across a Narrow Transmembrane Channel. Journal of Chemical Theory and Computation, 2021, 17, 1726-1741.	2.3	26
5	Insights into substrate recognition and specificity for IgG by Endoglycosidase S2. PLoS Computational Biology, 2021, 17, e1009103.	1.5	5
6	Development of CHARMM Additive Potential Energy Parameters for Î±-Methyl Amino Acids. Journal of Physical Chemistry B, 2021, 125, 11687-11696.	1.2	0
7	Improved Modeling of Cationâ€Ï€ and Anionâ€Ring Interactions Using the Drude Polarizable Empirical Force Field for Proteins. Journal of Computational Chemistry, 2020, 41, 439-448.	1.5	27
8	FFParam: Standalone package for CHARMM additive and Drude polarizable force field parametrization of small molecules. Journal of Computational Chemistry, 2020, 41, 958-970.	1.5	50
9	Statistical mechanics of polarizable force fields based on classical Drude oscillators with dynamical propagation by the dual-thermostat extended Lagrangian. Journal of Chemical Physics, 2020, 153, 114108.	1.2	11
10	Predicting Partition Coefficients of Neutral and Charged Solutes in the Mixed SLESâ€“Fatty Acid Micellar System. Journal of Physical Chemistry B, 2020, 124, 1653-1664.	1.2	5
11	Further Optimization and Validation of the Classical Drude Polarizable Protein Force Field. Journal of Chemical Theory and Computation, 2020, 16, 3221-3239.	2.3	53
12	Drude Polarizable Force Field Parametrization of Carboxylate and N-Acetyl Amine Carbohydrate Derivatives. Journal of Chemical Theory and Computation, 2019, 15, 4982-5000.	2.3	20
13	Molecular Dynamics Simulations of Ionic Liquids and Electrolytes Using Polarizable Force Fields. Chemical Reviews, 2019, 119, 7940-7995.	23.0	386
14	Toward Prediction of Electrostatic Parameters for Force Fields That Explicitly Treat Electronic Polarization. Journal of Chemical Theory and Computation, 2019, 15, 2460-2469.	2.3	21
15	Improved Modeling of Halogenated Ligandâ€“Protein Interactions Using the Drude Polarizable and CHARMM Additive Empirical Force Fields. Journal of Chemical Information and Modeling, 2019, 59, 215-228.	2.5	23
16	Polarizable Force Field for Molecular Ions Based on the Classical Drude Oscillator. Journal of Chemical Information and Modeling, 2018, 58, 993-1004.	2.5	45
17	Molecular dynamics simulations using the drude polarizable force field on GPUs with OpenMM: Implementation, validation, and benchmarks. Journal of Computational Chemistry, 2018, 39, 1682-1689.	1.5	77
18	CHARMM Drude Polarizable Force Field for Glycosidic Linkages Involving Pyranoses and Furanoses. Journal of Chemical Theory and Computation, 2018, 14, 3132-3143.	2.3	29

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19	Optimized Lennard-Jones Parameters for Druglike Small Molecules. Journal of Chemical Theory and Computation, 2018, 14, 3121-3131.	2.3	44
20	Polarizable force field for RNA based on the classical drude oscillator. Journal of Computational Chemistry, 2018, 39, 2624-2646.	1.5	67
21	Mapping the Drude polarizable force field onto a multipole and induced dipole model. Journal of Chemical Physics, 2017, 147, 161702.	1.2	42
22	<scp>DIRECTâ€ID</scp>: An automated method to identify and quantify conformational variationsâ€"application to Î²₂â€adrenergic <scp>GPCR</scp>. Journal of Computational Chemistry, 2016, 37, 416-425.	1.5	13
23	Additive <scp>CHARMM</scp> force field for naturally occurring modified ribonucleotides. Journal of Computational Chemistry, 2016, 37, 896-912.	1.5	63
24	Allâ€atom polarizable force field for DNA based on the classical drude oscillator model. Journal of Computational Chemistry, 2014, 35, 1219-1239.	1.5	136
25	CHARMM36 all-atom additive protein force field: Validation based on comparison to NMR data. Journal of Computational Chemistry, 2013, 34, 2135-2145.	1.5	2,613
26	Polarizable Empirical Force Field for Acyclic Polyalcohols Based on the Classical Drude Oscillator. Biopolymers, 2013, 99, 724-738.	1.2	50
27	Kirkwood-Buff analysis of aqueous N-methylacetamide and acetamide solutions modeled by the CHARMM additive and Drude polarizable force fields. Journal of Chemical Physics, 2013, 139, 084509.	1.2	31
28	Six-site polarizable model of water based on the classical Drude oscillator. Journal of Chemical Physics, 2013, 138, 034508.	1.2	103
29	Impact of Ribosomal Modification on the Binding of the Antibiotic Telithromycin Using a Combined Grand Canonical Monte Carlo/Molecular Dynamics Simulation Approach. PLoS Computational Biology, 2013, 9, e1003113.	1.5	18
30	Rapid estimation of hydration thermodynamics of macromolecular regions. Journal of Chemical Physics, 2013, 139, 055105.	1.2	19
31	(Ala)₄â€Â€(Ala)₄ as a model system for the optimization of the Ï‡₁ and Ï‡₂ amino acid sideâ€chain dihedral empirical force field parameters. Journal of Computational Chemistry, 2013, 34, 593-603.	1.5	5
32	Hydrophobic residues in small ankyrin 1 participate in binding to obscurin. Molecular Membrane Biology, 2012, 29, 36-51.	2.0	7
33	Recent developments and applications of the CHARMM force fields. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 167-185.	6.2	173
34	Balancing target flexibility and target denaturation in computational fragmentâ€based inhibitor discovery. Journal of Computational Chemistry, 2012, 33, 1880-1891.	1.5	36
35	Extension of the CHARMM general force field to sulfonylâ€containing compounds and its utility in biomolecular simulations. Journal of Computational Chemistry, 2012, 33, 2451-2468.	1.5	659
36	Structural mechanism associated with domain opening in gainâ€ofâ€function mutations in SHP2 phosphatase. Proteins: Structure, Function and Bioinformatics, 2011, 79, 1573-1588.	1.5	37

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37	Impact of 2â€²â€hydroxyl sampling on the conformational properties of RNA: Update of the CHARMM allâ€atom additive force field for RNA. Journal of Computational Chemistry, 2011, 32, 1929-1943.	1.5	341
38	Polarizable empirical force field for sulfurâ€containing compounds based on the classical Drude oscillator model. Journal of Computational Chemistry, 2010, 31, 2330-2341.	1.5	45
39	Computational Fragment-Based Binding Site Identification by Ligand Competitive Saturation. PLoS Computational Biology, 2009, 5, e1000435.	1.5	208
40	Polarizable empirical force field for nitrogenâ€containing heteroaromatic compounds based on the classical Drude oscillator. Journal of Computational Chemistry, 2009, 30, 1821-1838.	1.5	65
41	Additive empirical force field for hexopyranose monosaccharides. Journal of Computational Chemistry, 2008, 29, 2543-2564.	1.5	483
42	Development of a Polarizable Intermolecular Potential Function (PIPF) for Liquid Amides and Alkanes. Journal of Chemical Theory and Computation, 2007, 3, 1878-1889.	2.3	107
43	DNA bending induced by carbocyclic sugar analogs constrained to the north conformation. Biopolymers, 2007, 85, 438-449.	1.2	5
44	CHARMM force field parameters for simulation of reactive intermediates in native and thio-substituted ribozymes. Journal of Computational Chemistry, 2007, 28, 495-507.	1.5	49
45	CH/Ï€ interactions involving aromatic amino acids: Refinement of the CHARMM tryptophan force field. Journal of Computational Chemistry, 2005, 26, 1452-1463.	1.5	83
46	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, 1400-1415.	1.5	3,145
47	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, 1504-1514.	1.5	410
48	Empirical force fields for biological macromolecules: Overview and issues. Journal of Computational Chemistry, 2004, 25, 1584-1604.	1.5	1,134
49	The Structure of Aqueous Guanidinium Chloride Solutions. Journal of the American Chemical Society, 2004, 126, 11462-11470.	6.6	245
50	A simple polarizable model of water based on classical Drude oscillators. Journal of Chemical Physics, 2003, 119, 5185-5197.	1.2	635
51	Combinedab initio/empirical approach for optimization of Lennard-Jones parameters for polar-neutral compounds. Journal of Computational Chemistry, 2002, 23, 199-213.	1.5	100
52	Ab initio conformational analysis of nucleic acid components: Intrinsic energetic contributions to nucleic acid structure and dynamics. Biopolymers, 2001, 61, 61-76.	1.2	70
53	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.	1.5	701
54	Development and current status of the CHARMM force field for nucleic acids. Biopolymers, 2000, 56, 257-265.	1.2	923

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55	Combinedab initio/empirical approach for optimization of Lennard-Jones parameters. Journal of Computational Chemistry, 1998, 19, 334-348.	1.5	181