Justin A Lemkul

List of Publications by Year
in descending order

| 52 papers | 5,899 citations | 201674
27 h-index | 182427
51 g-index |
| 55 all docs | 55 docs citations | 55 times ranked | 7866 citing authors |

#	Article	IF	Citations
1	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, 405-413.	5.3	2,567
2	An Empirical Polarizable Force Field Based on the Classical Drude Oscillator Model: Development History and Recent Applications. Chemical Reviews, 2016, 116, 4983-5013.	47.7	434
3	Assessing the Stability of Alzheimer's Amyloid Protofibrils Using Molecular Dynamics. Journal of Physical Chemistry B, 2010, 114, 1652-1660.	2.6	398
4	GridMAT-MD: A grid-based membrane analysis tool for use with molecular dynamics. Journal of Computational Chemistry, 2009, 30, 1952-1958.	3.3	272
5	From Proteins to Perturbed Hamiltonians: A Suite of Tutorials for the GROMACS-2018 Molecular Simulation Package [Article v1.0]. Living Journal of Computational Molecular Science, 2019, 1, .	6.4	200
6	Practical Considerations for Building GROMOS-Compatible Small-Molecule Topologies. Journal of Chemical Information and Modeling, 2010, 50, 2221-2235.	5.4	180
7	Parametrization of halogen bonds in the CHARMM general force field: Improved treatment of ligand–protein interactions. Bioorganic and Medicinal Chemistry, 2016, 24, 4812-4825.	3.0	168
8	Destabilizing Alzheimer's Aβ_{42} Protofibrils with Morin: Mechanistic Insights from Molecular Dynamics Simulations. Biochemistry, 2010, 49, 3935-3946.	2.5	162
9	The Role of Molecular Simulations in the Development of Inhibitors of Amyloid β-Peptide Aggregation for the Treatment of Alzheimer's Disease. ACS Chemical Neuroscience, 2012, 3, 845-856.	3.5	98
10	Lipid composition influences the release of Alzheimer's amyloid β-peptide from membranes. Protein Science, 2011, 20, 1530-1545.	7.6	81
11	Implementation of extended Lagrangian dynamics in GROMACS for polarizable simulations using the classical Drude oscillator model. Journal of Computational Chemistry, 2015, 36, 1473-1479.	3.3	79
12	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.	3.3	77
13	Comparing atomistic molecular mechanics force fields for a difficult target: a case study on the Alzheimer's amyloid β-peptide. Journal of Biomolecular Structure and Dynamics, 2014, 32, 1817-1832.	3.5	74
14	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.	5.3	69
15	Polarizable Force Field for DNA Based on the Classical Drude Oscillator: I. Refinement Using Quantum Mechanical Base Stacking and Conformational Energetics. Journal of Chemical Theory and Computation, 2017, 13, 2053-2071.	5.3	68
16	Polarizable force field for RNA based on the classical drude oscillator. Journal of Computational Chemistry, 2018, 39, 2624-2646.	3.3	67
17	Perturbation of membranes by the amyloid β-peptide – a molecular dynamics study. FEBS Journal, 2009, 276, 3060-3075.	4.7	65
18	Morin Inhibits the Early Stages of Amyloid β-Peptide Aggregation by Altering Tertiary and Quaternary Interactions to Produce "Off-Pathway" Structures. Biochemistry, 2012, 51, 5990-6009.	2.5	64

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19	A comparative molecular dynamics analysis of the amyloid β-peptide in a lipid bilayer. Archives of Biochemistry and Biophysics, 2008, 470, 54-63.	3.0	62
20	Induced Polarization Influences the Fundamental Forces in DNA Base Flipping. Journal of Physical Chemistry Letters, 2014, 5, 2077-2083.	4.6	59
21	Same fold, different properties: polarizable molecular dynamics simulations of telomeric and TERRA G-quadruplexes. Nucleic Acids Research, 2020, 48, 561-575.	14.5	57
22	Aggregation of Alzheimer's Amyloid β-Peptide in Biological Membranes: A Molecular Dynamics Study. Biochemistry, 2013, 52, 4971-4980.	2.5	51
23	Characterization of Mg^{2+} Distributions around RNA in Solution. ACS Omega, 2016, 1, 680-688.	3.5	40
24	Balancing the Interactions of Mg^{2+} in Aqueous Solution and with Nucleic Acid Moieties For a Polarizable Force Field Based on the Classical Drude Oscillator Model. Journal of Physical Chemistry B, 2016, 120, 11436-11448.	2.6	37
25	Tyrosine aminotransferase: biochemical and structural properties and molecular dynamics simulations. Protein and Cell, 2010, 1, 1023-1032.	11.0	36
26	Molecular Dynamics Simulations of the *c-kit1* Promoter G-Quadruplex: Importance of Electronic Polarization on Stability and Cooperative Ion Binding. Journal of Physical Chemistry B, 2019, 123, 148-159.	2.6	34
27	Simulations of monomeric amyloid β-peptide (1–40) with varying solution conditions and oxidation state of Met35: Implications for aggregation. Archives of Biochemistry and Biophysics, 2014, 545, 44-52.	3.0	33
28	Induced Dipole–Dipole Interactions Influence the Unfolding Pathways of Wild-Type and Mutant Amyloid β-Peptides. Journal of Physical Chemistry B, 2015, 119, 15574-15582.	2.6	30
29	Structure and Dynamics of FosA-Mediated Fosfomycin Resistance in Klebsiella pneumoniae and Escherichia coli. Antimicrobial Agents and Chemotherapy, 2017, 61, .	3.2	28
30	Recent developments in empirical atomistic force fields for nucleic acids and applications to studies of folding and dynamics. Current Opinion in Structural Biology, 2021, 67, 9-17.	5.7	28
31	Insights into Stabilizing Forces in Amyloid Fibrils of Differing Sizes from Polarizable Molecular Dynamics Simulations. Journal of Molecular Biology, 2018, 430, 3819-3834.	4.2	26
32	Small Molecule Thermochemistry: A Tool for Empirical Force Field Development. Journal of Physical Chemistry A, 2018, 122, 8982-8988.	2.5	25
33	Polarizable Molecular Dynamics Simulations of Two *c-kit* Oncogene Promoter G-Quadruplexes: Effect of Primary and Secondary Structure on Loop and Ion Sampling. Journal of Chemical Theory and Computation, 2020, 16, 3430-3444.	5.3	24
34	CHARMM-GUI Drude prepper for molecular dynamics simulation using the classical Drude polarizable force field. Journal of Computational Chemistry, 2022, 43, 359-375.	3.3	24
35	Biophysical and Molecular-Dynamics Studies of Phosphatidic Acid Binding by the Dvl-2 DEP Domain. Biophysical Journal, 2014, 106, 1101-1111.	0.5	23
36	Characterization of Interactions between PilA from Pseudomonas aeruginosa Strain K and a Model Membrane. Journal of Physical Chemistry B, 2011, 115, 8004-8008.	2.6	21

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37	Pairwise-additive and polarizable atomistic force fields for molecular dynamics simulations of proteins. Progress in Molecular Biology and Translational Science, 2020, 170, 1-71.	1.7	16
38	Phosphorylation of PPARÎ³ Affects the Collective Motions of the PPARÎ³-RXRÎ±-DNA Complex. PLoS ONE, 2015, 10, e0123984.	2.5	15
39	<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.	3.3	13
40	HIV-1 Env gp41 Transmembrane Domain Dynamics Are Modulated by Lipid, Water, and Ion Interactions. Biophysical Journal, 2018, 115, 84-94.	0.5	13
41	FusoPortal: an Interactive Repository of Hybrid MinION-Sequenced <i>Fusobacterium</i> Genomes Improves Gene Identification and Characterization. MSphere, 2018, 3, .	2.9	12
42	Sequential Bending and Twisting around Câ€"C Single Bonds by Mechanical Lifting of a Pre-Adsorbed Polymer. Nano Letters, 2020, 20, 652-657.	9.1	12
43	Integration of experimental data and use of automated fitting methods in developing protein force fields. Communications Chemistry, 2022, 5, .	4.5	12
44	<scp>TUPÃƒ</scp>: Electric field analyses for molecular simulations. Journal of Computational Chemistry, 2022, 43, 1113-1119.	3.3	9
45	Ion Binding Properties and Dynamics of the <i>bcl-</i>2 G-Quadruplex Using a Polarizable Force Field. Journal of Chemical Information and Modeling, 2020, 60, 6476-6488.	5.4	7
46	Complete Genome Sequence of Fusobacterium necrophorum subsp. necrophorum ATCC 25286. Microbiology Resource Announcements, 2019, 8, .	0.6	5
47	Cation competition and recruitment around the c-kit1 G-quadruplex using polarizable simulations. Biophysical Journal, 2021, 120, 2249-2261.	0.5	5
48	Impact of Electronic Polarization on Preformed, Î²-Strand Rich Homogenous and Heterogenous Amyloid Oligomers. Journal of Computational Biophysics and Chemistry, 0, , .	1.7	5
49	Ion-Dependent Conformational Plasticity of Telomeric G-Hairpins and G-Quadruplexes. ACS Omega, 2022, 7, 23368-23379.	3.5	5
50	Preparing and Analyzing Polarizable Molecular Dynamics Simulations with the Classical Drude Oscillator Model. Methods in Molecular Biology, 2021, 2315, 219-240.	0.9	2
51	Polarizable Molecular Dynamics Simulations of C-Kit Oncogene Promoter G-Quadruplexes of Distinct Conformations. Biophysical Journal, 2019, 116, 360a.	0.5	1
52	Electronic Polarization at the Interface between the p53 Transactivation Domain and Two Binding Partners. Journal of Physical Chemistry B, 0, , .	2.6	1