

# Justin A Lemkul

## List of Publications by Year in descending order

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Version: 2024-02-01

52  
papers

5,899  
citations

201575

27  
h-index

182361

51  
g-index

55  
all docs

55  
docs citations

55  
times ranked

7866  
citing authors

#	ARTICLE	IF	CITATIONS
1	Integration of experimental data and use of automated fitting methods in developing protein force fields. <i>Communications Chemistry</i> , 2022, 5, .	2.0	12
2	<sc>CHARMMâ€GUI</sc> 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
3	<sc>TUPÃf</sc>: Electric field analyses for molecular simulations. <i>Journal of Computational Chemistry</i> , 2022, 43, 1113-1119.	1.5	9
4	Ion-Dependent Conformational Plasticity of Telomeric G-Hairpins and G-Quadruplexes. <i>ACS Omega</i> , 2022, 7, 23368-23379.	1.6	5
5	Recent developments in empirical atomistic force fields for nucleic acids and applications to studies of folding and dynamics. <i>Current Opinion in Structural Biology</i> , 2021, 67, 9-17.	2.6	28
6	Cation competition and recruitment around the c-kit1 G-quadruplex using polarizable simulations. <i>Biophysical Journal</i> , 2021, 120, 2249-2261.	0.2	5
7	Preparing and Analyzing Polarizable Molecular Dynamics Simulations with the Classical Drude Oscillator Model. <i>Methods in Molecular Biology</i> , 2021, 2315, 219-240.	0.4	2
8	Sequential Bending and Twisting around Câ€C Single Bonds by Mechanical Lifting of a Pre-Adsorbed Polymer. <i>Nano Letters</i> , 2020, 20, 652-657.	4.5	12
9	Same fold, different properties: polarizable molecular dynamics simulations of telomeric and TERRA G-quadruplexes. <i>Nucleic Acids Research</i> , 2020, 48, 561-575.	6.5	57
10	Ion Binding Properties and Dynamics of the <i>bcl</i>2 G-Quadruplex Using a Polarizable Force Field. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 6476-6488.	2.5	7
11	Pairwise-additive and polarizable atomistic force fields for molecular dynamics simulations of proteins. <i>Progress in Molecular Biology and Translational Science</i> , 2020, 170, 1-71.	0.9	16
12	Polarizable Molecular Dynamics Simulations of Two <i>c-kit</i> Oncogene Promoter G-Quadruplexes: Effect of Primary and Secondary Structure on Loop and Ion Sampling. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3430-3444.	2.3	24
13	Polarizable Molecular Dynamics Simulations of C-Kit Oncogene Promoter G-Quadruplexes of Distinct Conformations. <i>Biophysical Journal</i> , 2019, 116, 360a.	0.2	1
14	Complete Genome Sequence of <i>Fusobacterium necrophorum</i> subsp. <i>necrophorum</i> ATCC 25286. <i>Microbiology Resource Announcements</i> , 2019, 8, .	0.3	5
15	Molecular Dynamics Simulations of the <i>c-kit1</i> Promoter G-Quadruplex: Importance of Electronic Polarization on Stability and Cooperative Ion Binding. <i>Journal of Physical Chemistry B</i> , 2019, 123, 148-159.	1.2	34
16	From Proteins to Perturbed Hamiltonians: A Suite of Tutorials for the GROMACS-2018 Molecular Simulation Package [Article v1.0]. <i>Living Journal of Computational Molecular Science</i> , 2019, 1, .	2.2	200
17	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
18	Polarizable force field for RNA based on the classical drude oscillator. <i>Journal of Computational Chemistry</i> , 2018, 39, 2624-2646.	1.5	67

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19	Small Molecule Thermochemistry: A Tool for Empirical Force Field Development. <i>Journal of Physical Chemistry A</i> , 2018, 122, 8982-8988.	1.1	25
20	Insights into Stabilizing Forces in Amyloid Fibrils of Differing Sizes from Polarizable Molecular Dynamics Simulations. <i>Journal of Molecular Biology</i> , 2018, 430, 3819-3834.	2.0	26
21	HIV-1 Env gp41 Transmembrane Domain Dynamics Are Modulated by Lipid, Water, and Ion Interactions. <i>Biophysical Journal</i> , 2018, 115, 84-94.	0.2	13
22	FusoPortal: an Interactive Repository of Hybrid MinION-Sequenced <i>Fusobacterium</i> Genomes Improves Gene Identification and Characterization. <i>MSphere</i> , 2018, 3, .	1.3	12
23	Polarizable Force Field for DNA Based on the Classical Drude Oscillator: I. Refinement Using Quantum Mechanical Base Stacking and Conformational Energetics. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2053-2071.	2.3	68
24	Polarizable Force Field for DNA Based on the Classical Drude Oscillator: II. Microsecond Molecular Dynamics Simulations of Duplex DNA. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2072-2085.	2.3	69
25	Structure and Dynamics of FosA-Mediated Fosfomycin Resistance in <i>Klebsiella pneumoniae</i> and <i>Escherichia coli</i> . <i>Antimicrobial Agents and Chemotherapy</i> , 2017, 61, .	1.4	28
26	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
27	Characterization of $Mg^{2+}$ Distributions around RNA in Solution. <i>ACS Omega</i> , 2016, 1, 680-688.	1.6	40
28	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. <i>Journal of Physical Chemistry B</i> , 2016, 120, 11436-11448.	1.2	37
29	Parametrization of halogen bonds in the CHARMM general force field: Improved treatment of ligand-protein interactions. <i>Bioorganic and Medicinal Chemistry</i> , 2016, 24, 4812-4825.	1.4	168
30	An Empirical Polarizable Force Field Based on the Classical Drude Oscillator Model: Development History and Recent Applications. <i>Chemical Reviews</i> , 2016, 116, 4983-5013.	23.0	434
31	CHARMM-GUI Input Generator for NAMD, GROMACS, AMBER, OpenMM, and CHARMM/OpenMM Simulations Using the CHARMM36 Additive Force Field. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 405-413.	2.3	2,567
32	Implementation of extended Lagrangian dynamics in GROMACS for polarizable simulations using the classical Drude oscillator model. <i>Journal of Computational Chemistry</i> , 2015, 36, 1473-1479.	1.5	79
33	Induced Dipole-Dipole Interactions Influence the Unfolding Pathways of Wild-Type and Mutant Amyloid $\beta$ -Peptides. <i>Journal of Physical Chemistry B</i> , 2015, 119, 15574-15582.	1.2	30
34	Phosphorylation of PPAR $\beta$ Affects the Collective Motions of the PPAR $\beta$ -RXR $\beta$ -DNA Complex. <i>PLoS ONE</i> , 2015, 10, e0123984.	1.1	15
35	Comparing atomistic molecular mechanics force fields for a difficult target: a case study on the Alzheimer's amyloid $\beta$ -peptide. <i>Journal of Biomolecular Structure and Dynamics</i> , 2014, 32, 1817-1832.	2.0	74
36	Biophysical and Molecular-Dynamics Studies of Phosphatidic Acid Binding by the Dvl-2 DEP Domain. <i>Biophysical Journal</i> , 2014, 106, 1101-1111.	0.2	23

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37	Simulations of monomeric amyloid $\beta$ -peptide (1-40) with varying solution conditions and oxidation state of Met35: Implications for aggregation. Archives of Biochemistry and Biophysics, 2014, 545, 44-52.	1.4	33
38	Induced Polarization Influences the Fundamental Forces in DNA Base Flipping. Journal of Physical Chemistry Letters, 2014, 5, 2077-2083.	2.1	59
39	Aggregation of Alzheimer's Amyloid $\beta$ -Peptide in Biological Membranes: A Molecular Dynamics Study. Biochemistry, 2013, 52, 4971-4980.	1.2	51
40	Morin Inhibits the Early Stages of Amyloid $\beta$ -Peptide Aggregation by Altering Tertiary and Quaternary Interactions to Produce "Off-Pathway" Structures. Biochemistry, 2012, 51, 5990-6009.	1.2	64
41	The Role of Molecular Simulations in the Development of Inhibitors of Amyloid $\beta$ -Peptide Aggregation for the Treatment of Alzheimer's Disease. ACS Chemical Neuroscience, 2012, 3, 845-856.	1.7	98
42	Characterization of Interactions between PilA from Pseudomonas aeruginosa Strain K and a Model Membrane. Journal of Physical Chemistry B, 2011, 115, 8004-8008.	1.2	21
43	Lipid composition influences the release of Alzheimer's amyloid $\beta$ -peptide from membranes. Protein Science, 2011, 20, 1530-1545.	3.1	81
44	Destabilizing Alzheimer's $\beta$ -Protofibrils with Morin: Mechanistic Insights from Molecular Dynamics Simulations. Biochemistry, 2010, 49, 3935-3946.	1.2	162
45	Practical Considerations for Building GROMOS-Compatible Small-Molecule Topologies. Journal of Chemical Information and Modeling, 2010, 50, 2221-2235.	2.5	180
46	Tyrosine aminotransferase: biochemical and structural properties and molecular dynamics simulations. Protein and Cell, 2010, 1, 1023-1032.	4.8	36
47	Assessing the Stability of Alzheimer's Amyloid Protofibrils Using Molecular Dynamics. Journal of Physical Chemistry B, 2010, 114, 1652-1660.	1.2	398
48	GridMAT-MD: A grid-based membrane analysis tool for use with molecular dynamics. Journal of Computational Chemistry, 2009, 30, 1952-1958.	1.5	272
49	Perturbation of membranes by the amyloid $\beta$ -peptide " a molecular dynamics study. FEBS Journal, 2009, 276, 3060-3075.	2.2	65
50	A comparative molecular dynamics analysis of the amyloid $\beta$ -peptide in a lipid bilayer. Archives of Biochemistry and Biophysics, 2008, 470, 54-63.	1.4	62
51	Impact of Electronic Polarization on Preformed, $\beta$ -Strand Rich Homogenous and Heterogenous Amyloid Oligomers. Journal of Computational Biophysics and Chemistry, 0, , .	1.0	5
52	Electronic Polarization at the Interface between the p53 Transactivation Domain and Two Binding Partners. Journal of Physical Chemistry B, 0, , .	1.2	1