Justin A Lemkul

List of Publications by Year
in descending order

52 papers	5,899 citations	201658 27 h-index	182417 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. Communications Chemistry, 2022, 5, .	4.5	12
2	<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.	3.3	24
3	<scp>TUPÃƒ</scp>: Electric field analyses for molecular simulations. Journal of Computational Chemistry, 2022, 43, 1113-1119.	3.3	9
4	Ion-Dependent Conformational Plasticity of Telomeric G-Hairpins and G-Quadruplexes. ACS Omega, 2022, 7, 23368-23379.	3.5	5
5	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
6	Cation competition and recruitment around the c-kit1 G-quadruplex using polarizable simulations. Biophysical Journal, 2021, 120, 2249-2261.	0.5	5
7	Preparing and Analyzing Polarizable Molecular Dynamics Simulations with the Classical Drude Oscillator Model. Methods in Molecular Biology, 2021, 2315, 219-240.	0.9	2
8	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
9	Same fold, different properties: polarizable molecular dynamics simulations of telomeric and TERRA G-quadruplexes. Nucleic Acids Research, 2020, 48, 561-575.	14.5	57
10	Ion Binding Properties and Dynamics of the bcl-2 G-Quadruplex Using a Polarizable Force Field. Journal of Chemical Information and Modeling, 2020, 60, 6476-6488.	5.4	7
11	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
12	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
13	Polarizable Molecular Dynamics Simulations of C-Kit Oncogene Promoter G-Quadruplexes of Distinct Conformations. Biophysical Journal, 2019, 116, 360a.	0.5	1
14	Complete Genome Sequence of Fusobacterium necrophorum subsp. necrophorum ATCC 25286. Microbiology Resource Announcements, 2019, 8, .	0.6	5
15	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
16	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
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.	3.3	77
18	Polarizable force field for RNA based on the classical drude oscillator. Journal of Computational Chemistry, 2018, 39, 2624-2646.	3.3	67

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19	Small Molecule Thermochemistry: A Tool for Empirical Force Field Development. Journal of Physical Chemistry A, 2018, 122, 8982-8988.	2.5	25
20	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
21	HIV-1 Env gp41 Transmembrane Domain Dynamics Are Modulated by Lipid, Water, and Ion Interactions. Biophysical Journal, 2018, 115, 84-94.	0.5	13
22	FusoPortal: an Interactive Repository of Hybrid MinION-Sequenced Fusobacterium Genomes Improves Gene Identification and Characterization. MSphere, 2018, 3, .	2.9	12
23	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
24	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
25	Structure and Dynamics of FosA-Mediated Fosfomycin Resistance in Klebsiella pneumoniae and Escherichia coli. Antimicrobial Agents and Chemotherapy, 2017, 61, .	3.2	28
26	<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
27	Characterization of Mg²⁺ Distributions around RNA in Solution. ACS Omega, 2016, 1, 680-688.	3.5	40
28	Balancing the Interactions of Mg²⁺ 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
29	Parametrization of halogen bonds in the CHARMM general force field: Improved treatment of ligandâ€"protein interactions. Bioorganic and Medicinal Chemistry, 2016, 24, 4812-4825.	3.0	168
30	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
31	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
32	Implementation of extended <scp>L</scp>agrangian dynamics in <scp>GROMACS</scp> for polarizable simulations using the classical <scp>D</scp>rude oscillator model. Journal of Computational Chemistry, 2015, 36, 1473-1479.	3.3	79
33	Induced Dipoleâ€"Dipole Interactions Influence the Unfolding Pathways of Wild-Type and Mutant Amyloid Î²-Peptides. Journal of Physical Chemistry B, 2015, 119, 15574-15582.	2.6	30
34	Phosphorylation of PPARÎ³ Affects the Collective Motions of the PPARÎ³-RXRÎ±-DNA Complex. PLoS ONE, 2015, 10, e0123984.	2.5	15
35	Comparing atomistic molecular mechanics force fields for a difficult target: a case study on the Alzheimerâ€™s amyloid Î²-peptide. Journal of Biomolecular Structure and Dynamics, 2014, 32, 1817-1832.	3.5	74
36	Biophysical and Molecular-Dynamics Studies of Phosphatidic Acid Binding by the Dvl-2 DEP Domain. Biophysical Journal, 2014, 106, 1101-1111.	0.5	23

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37	Simulations of monomeric amyloid Î²-peptide (1â€“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
38	Induced Polarization Influences the Fundamental Forces in DNA Base Flipping. Journal of Physical Chemistry Letters, 2014, 5, 2077-2083.	4.6	59
39	Aggregation of Alzheimerâ€™s Amyloid Î²-Peptide in Biological Membranes: A Molecular Dynamics Study. Biochemistry, 2013, 52, 4971-4980.	2.5	51
40	Morin Inhibits the Early Stages of Amyloid Î²-Peptide Aggregation by Altering Tertiary and Quaternary Interactions to Produce â€œOff-Pathwayâ€•Structures. Biochemistry, 2012, 51, 5990-6009.	2.5	64
41	The Role of Molecular Simulations in the Development of Inhibitors of Amyloid Î²-Peptide Aggregation for the Treatment of Alzheimerâ€™s Disease. ACS Chemical Neuroscience, 2012, 3, 845-856.	3.5	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.	2.6	21
43	Lipid composition influences the release of Alzheimer's amyloid Î²â€peptide from membranes. Protein Science, 2011, 20, 1530-1545.	7.6	81
44	Destabilizing Alzheimerâ€™s AÎ²₄₂Protofibrils with Morin: Mechanistic Insights from Molecular Dynamics Simulations. Biochemistry, 2010, 49, 3935-3946.	2.5	162
45	Practical Considerations for Building GROMOS-Compatible Small-Molecule Topologies. Journal of Chemical Information and Modeling, 2010, 50, 2221-2235.	5.4	180
46	Tyrosine aminotransferase: biochemical and structural properties and molecular dynamics simulations. Protein and Cell, 2010, 1, 1023-1032.	11.0	36
47	Assessing the Stability of Alzheimerâ€™s Amyloid Protofibrils Using Molecular Dynamics. Journal of Physical Chemistry B, 2010, 114, 1652-1660.	2.6	398
48	GridMATâ€MD: A gridâ€based membrane analysis tool for use with molecular dynamics. Journal of Computational Chemistry, 2009, 30, 1952-1958.	3.3	272
49	Perturbation of membranes by the amyloid Î²â€peptide â€“ a molecular dynamics study. FEBS Journal, 2009, 276, 3060-3075.	4.7	65
50	A comparative molecular dynamics analysis of the amyloid Î²-peptide in a lipid bilayer. Archives of Biochemistry and Biophysics, 2008, 470, 54-63.	3.0	62
51	Impact of Electronic Polarization on Preformed, Î²-Strand Rich Homogenous and Heterogenous Amyloid Oligomers. Journal of Computational Biophysics and Chemistry, 0, , .	1.7	5
52	Electronic Polarization at the Interface between the p53 Transactivation Domain and Two Binding Partners. Journal of Physical Chemistry B, 0, , .	2.6	1