# Justin A Lemkul

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/795299/publications.pdf

Version: 2024-02-01

| 52 | 5,899 | 201575 27 | 182361 51 |
|---|---|---|---|
| papers | citations | h-index | g-index |

| 55 | 55 | 55 | 7866 |
|---|---|---|---|
| all docs | docs citations | times ranked | 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. | 2.3 | 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. | 23.0 | 434 |
| 3 | Assessing the Stability of Alzheimerâ€™s Amyloid Protofibrils Using Molecular Dynamics. Journal of Physical Chemistry B, 2010, 114, 1652-1660. | 1.2 | 398 |
| 4 | GridMATâ€MD: A gridâ€based membrane analysis tool for use with molecular dynamics. Journal of Computational Chemistry, 2009, 30, 1952-1958. | 1.5 | 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, . | 2.2 | 200 |
| 6 | Practical Considerations for Building GROMOS-Compatible Small-Molecule Topologies. Journal of Chemical Information and Modeling, 2010, 50, 2221-2235. | 2.5 | 180 |
| 7 | Parametrization of halogen bonds in the CHARMM general force field: Improved treatment of ligandâ€“protein interactions. Bioorganic and Medicinal Chemistry, 2016, 24, 4812-4825. | 1.4 | 168 |
| 8 | Destabilizing Alzheimerâ€™s AÎ²<sub>42</sub>Protofibrils with Morin: Mechanistic Insights from Molecular Dynamics Simulations. Biochemistry, 2010, 49, 3935-3946. | 1.2 | 162 |
| 9 | 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. | 1.7 | 98 |
| 10 | Lipid composition influences the release of Alzheimer's amyloid Î²â€peptide from membranes. Protein Science, 2011, 20, 1530-1545. | 3.1 | 81 |
| 11 | 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. | 1.5 | 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. | 1.5 | 77 |
| 13 | 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. | 2.0 | 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. | 2.3 | 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. | 2.3 | 68 |
| 16 | Polarizable force field for RNA based on the classical drude oscillator. Journal of Computational Chemistry, 2018, 39, 2624-2646. | 1.5 | 67 |
| 17 | Perturbation of membranes by the amyloid Î²â€peptide â€“ a molecular dynamics study. FEBS Journal, 2009, 276, 3060-3075. | 2.2 | 65 |
| 18 | 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. | 1.2 | 64 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | A comparative molecular dynamics analysis of the amyloid Î²-peptide in a lipid bilayer. Archives of Biochemistry and Biophysics, 2008, 470, 54-63. | 1.4 | 62 |
| 20 | Induced Polarization Influences the Fundamental Forces in DNA Base Flipping. Journal of Physical Chemistry Letters, 2014, 5, 2077-2083. | 2.1 | 59 |
| 21 | Same fold, different properties: polarizable molecular dynamics simulations of telomeric and TERRA G-quadruplexes. Nucleic Acids Research, 2020, 48, 561-575. | 6.5 | 57 |
| 22 | Aggregation of Alzheimerâ€™s Amyloid Î²-Peptide in Biological Membranes: A Molecular Dynamics Study. Biochemistry, 2013, 52, 4971-4980. | 1.2 | 51 |
| 23 | Characterization of Mg<sup>2+</sup> Distributions around RNA in Solution. ACS Omega, 2016, 1, 680-688. | 1.6 | 40 |
| 24 | Balancing the Interactions of Mg<sup>2+</sup> 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. | 1.2 | 37 |
| 25 | Tyrosine aminotransferase: biochemical and structural properties and molecular dynamics simulations. Protein and Cell, 2010, 1, 1023-1032. | 4.8 | 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. | 1.2 | 34 |
| 27 | 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. | 1.4 | 33 |
| 28 | 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. | 1.2 | 30 |
| 29 | Structure and Dynamics of FosA-Mediated Fosfomycin Resistance in Klebsiella pneumoniae and Escherichia coli. Antimicrobial Agents and Chemotherapy, 2017, 61, . | 1.4 | 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. | 2.6 | 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. | 2.0 | 26 |
| 32 | Small Molecule Thermochemistry: A Tool for Empirical Force Field Development. Journal of Physical Chemistry A, 2018, 122, 8982-8988. | 1.1 | 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. | 2.3 | 24 |
| 34 | <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 |
| 35 | Biophysical and Molecular-Dynamics Studies of Phosphatidic Acid Binding by the Dvl-2 DEP Domain. Biophysical Journal, 2014, 106, 1101-1111. | 0.2 | 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. | 1.2 | 21 |

| # | Article | IF | Citations |
|---|---|---|---|
| 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. | 0.9 | 16 |
| 38 | Phosphorylation of PPARÎ³ Affects the Collective Motions of the PPARÎ³-RXRÎ±-DNA Complex. PLoS ONE, 2015, 10, e0123984. | 1.1 | 15 |
| 39 | <scp>DIRECTâ€ID</scp>: An automated method to identify and quantify conformational variationsâ€”application to Î²<sub>2</sub>â€adrenergic <scp>GPCR</scp>. Journal of Computational Chemistry, 2016, 37, 416-425. | 1.5 | 13 |
| 40 | HIV-1 Env gp41 Transmembrane Domain Dynamics Are Modulated by Lipid, Water, and Ion Interactions. Biophysical Journal, 2018, 115, 84-94. | 0.2 | 13 |
| 41 | FusoPortal: an Interactive Repository of Hybrid MinION-Sequenced Fusobacterium Genomes Improves Gene Identification and Characterization. MSphere, 2018, 3, . | 1.3 | 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. | 4.5 | 12 |
| 43 | Integration of experimental data and use of automated fitting methods in developing protein force fields. Communications Chemistry, 2022, 5, . | 2.0 | 12 |
| 44 | <scp>TUPÃƒ</scp>: Electric field analyses for molecular simulations. Journal of Computational Chemistry, 2022, 43, 1113-1119. | 1.5 | 9 |
| 45 | 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. | 2.5 | 7 |
| 46 | Complete Genome Sequence of Fusobacterium necrophorum subsp. necrophorum ATCC 25286. Microbiology Resource Announcements, 2019, 8, . | 0.3 | 5 |
| 47 | Cation competition and recruitment around the c-kit1 G-quadruplex using polarizable simulations. Biophysical Journal, 2021, 120, 2249-2261. | 0.2 | 5 |
| 48 | Impact of Electronic Polarization on Preformed, Î²-Strand Rich Homogenous and Heterogenous Amyloid Oligomers. Journal of Computational Biophysics and Chemistry, 0, , . | 1.0 | 5 |
| 49 | Ion-Dependent Conformational Plasticity of Telomeric G-Hairpins and G-Quadruplexes. ACS Omega, 2022, 7, 23368-23379. | 1.6 | 5 |
| 50 | Preparing and Analyzing Polarizable Molecular Dynamics Simulations with the Classical Drude Oscillator Model. Methods in Molecular Biology, 2021, 2315, 219-240. | 0.4 | 2 |
| 51 | Polarizable Molecular Dynamics Simulations of C-Kit Oncogene Promoter G-Quadruplexes of Distinct Conformations. Biophysical Journal, 2019, 116, 360a. | 0.2 | 1 |
| 52 | Electronic Polarization at the Interface between the p53 Transactivation Domain and Two Binding Partners. Journal of Physical Chemistry B, 0, , . | 1.2 | 1 |