Guillaume Lamoureux

List of Publications by Year
in descending order

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38	4,030	331538	330025
papers	citations	21 h-index	37 g-index

39	39	39	3571
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Genetic, Structural, and Functional Evidence Link TMEM175 to Synucleinopathies. Annals of Neurology, 2020, 87, 139-153.	2.8	65
2	Drude polarizable force field for cationâ€“Ï€ interactions of alkali and quaternary ammonium ions with aromatic amino acid side chains. Journal of Computational Chemistry, 2020, 41, 472-481.	1.5	8
3	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
4	Salt-Dependent Interactions between the C-Terminal Domain of Osmoregulatory Transporter ProP of Escherichia coli and the Lipid Membrane. Journal of Physical Chemistry B, 2020, 124, 8209-8220.	1.2	5
5	The Impact of Composition and Morphology on Ionic Conductivity of Silk/Cellulose Bio-Composites Fabricated from Ionic Liquid and Varying Percentages of Coagulation Agents. International Journal of Molecular Sciences, 2020, 21, 4695.	1.8	19
6	Morphology and ionic conductivity relationship in silk/cellulose biocomposites. Polymer International, 2019, 68, 1580-1590.	1.6	17
7	Cationâ€Ï€ Interactions between Quaternary Ammonium Ions and Amino Acid Aromatic Groups in Aqueous Solution. Journal of Physical Chemistry B, 2018, 122, 2251-2260.	1.2	27
8	Dual Role of the C-Terminal Domain in Osmosensing by Bacterial Osmolyte Transporter ProP. Biophysical Journal, 2018, 115, 2152-2166.	0.2	11
9	Deep convolutional networks for quality assessment of protein folds. Bioinformatics, 2018, 34, 4046-4053.	1.8	69
10	Mechanism of the Nitric Oxide Dioxygenase Reaction of Mycobacterium tuberculosis Hemoglobin N. Journal of Physical Chemistry B, 2017, 121, 8706-8718.	1.2	12
11	Substrate-Specific Screening for Mutational Hotspots Using Biased Molecular Dynamics Simulations. ACS Catalysis, 2017, 7, 6786-6797.	5.5	17
12	Evolution of P450 Monooxygenases toward Formation of Transient Channels and Exclusion of Nonproductive Gases. ACS Catalysis, 2016, 6, 7426-7437.	5.5	14
13	Effect of Saturated Very Long-Chain Fatty Acids on the Organization of Lipid Membranes: A Study Combining ²H NMR Spectroscopy and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2016, 120, 6951-6960.	1.2	21
14	Three-dimensional structure model and predicted ATP interaction rewiring of a deviant RNA ligase 2. BMC Structural Biology, 2015, 15, 20.	2.3	4
15	Mechanism of NH 4 + Recruitment and NH 3 Transport in Rh Proteins. Structure, 2015, 23, 1550-1557.	1.6	27
16	Molecular Model of Hemoglobin N from Mycobacterium tuberculosis Bound to Lipid Bilayers: A Combined Spectroscopic and Computational Study. Biochemistry, 2015, 54, 2073-2084.	1.2	14
17	Identification of a Cholesterol-Binding Pocket in Inward Rectifier K + (Kir) Channels. Biophysical Journal, 2014, 107, 2786-2796.	0.2	28
18	Development of Semiempirical Models for Proton Transfer Reactions in Water. Journal of Chemical Theory and Computation, 2014, 10, 2881-2890.	2.3	8

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19	Simulation of Liquid and Supercritical Hydrogen Sulfide and of Alkali Ions in the Pure and Aqueous Liquid. Journal of Chemical Theory and Computation, 2014, 10, 3221-3235.	2.3	17
20	Different Hydration Patterns in the Pores of AmtB and RhCG Could Determine Their Transport Mechanisms. Biochemistry, 2013, 52, 7091-7098.	1.2	10
21	Polarizable Interaction Model for Liquid, Supercritical, and Aqueous Ammonia. Journal of Chemical Theory and Computation, 2013, 9, 2035-2051.	2.3	20
22	Molecular Dynamics Investigation of Alkali Metal Ions in Liquid and Aqueous Ammonia. Journal of Chemical Theory and Computation, 2013, 9, 2324-2338.	2.3	25
23	Molecular modelling of cationâ€“Ï€ interactions. Molecular Simulation, 2012, 38, 704-722.	0.9	23
24	Cationâˆ’Ï€ and Ï€â€“Ï€ Interactions in Aqueous Solution Studied Using Polarizable Potential Models. Journal of Chemical Theory and Computation, 2012, 8, 182-193.	2.3	62
25	Ammonium Transporters Achieve Charge Transfer by Fragmenting Their Substrate. Journal of the American Chemical Society, 2012, 134, 10419-10427.	6.6	60
26	Simulating Monovalent and Divalent Ions in Aqueous Solution Using a Drude Polarizable Force Field. Journal of Chemical Theory and Computation, 2010, 6, 774-786.	2.3	401
27	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
28	Reorganization free energies and quantum corrections for a model electron self-exchange reaction: comparison of polarizable and non-polarizable solvent models. Molecular Physics, 2008, 106, 1597-1611.	0.8	59
29	Computational Enzymology: Promises and Challenges. 2008 22nd International Symposium on High Performance Computing Systems and Applications, 2008, , .	0.0	0
30	Peptide Hydrolysis in Thermolysin:â€‰ Ab Initio QM/MM Investigation of the Glu143-Assisted Water Addition Mechanism. Journal of Chemical Theory and Computation, 2007, 3, 1837-1850.	2.3	60
31	Polarizable Empirical Force Field for Aromatic Compounds Based on the Classical Drude Oscillator. Journal of Physical Chemistry B, 2007, 111, 2873-2885.	1.2	149
32	A Stable Water Chain in the Hydrophobic Pore of the AmtB Ammonium Transporter. Biophysical Journal, 2007, 92, L82-L84.	0.2	37
33	Absolute Hydration Free Energy Scale for Alkali and Halide Ions Established from Simulations with a Polarizable Force Field. Journal of Physical Chemistry B, 2006, 110, 3308-3322.	1.2	357
34	A polarizable model of water for molecular dynamics simulations of biomolecules. Chemical Physics Letters, 2006, 418, 245-249.	1.2	548
35	Determination of Electrostatic Parameters for a Polarizable Force Field Based on the Classical Drude Oscillator. Journal of Chemical Theory and Computation, 2005, 1, 153-168.	2.3	260
36	Molecular Dynamics Study of Hydration in Ethanolâ€Water Mixtures Using a Polarizable Force Fieldâ€. Journal of Physical Chemistry B, 2005, 109, 6705-6713.	1.2	275

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37	A simple polarizable model of water based on classical Drude oscillators. Journal of Chemical Physics, 2003, 119, 5185-5197.	1.2	635
38	Modeling induced polarization with classical Drude oscillators: Theory and molecular dynamics simulation algorithm. Journal of Chemical Physics, 2003, 119, 3025-3039.	1.2	584