

Dirk Gillespie

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/7565110/publications.pdf>

Version: 2024-02-01

94
papers

4,208
citations

93792

39
h-index

129628

63
g-index

96
all docs

96
docs citations

96
times ranked

2806
citing authors

#	ARTICLE	IF	CITATIONS
1	Individual ion species chemical potentials in the Mean Spherical Approximation. Journal of Chemical Physics, 2022, 156, .	1.2	6
2	Physical interpretation of theories of homogeneous electrolytes in the primitive model. Journal of Molecular Liquids, 2022, 362, 119785.	2.3	3
3	Simulating cardiac Ca ²⁺ release units: effects of RyR cluster size and Ca ²⁺ buffers on diastolic Ca ²⁺ leak. Pflugers Archiv European Journal of Physiology, 2021, 473, 435-446.	1.3	5
4	Revisiting the Charged Shell Model: A Density Functional Theory for Electrolytes. Journal of Chemical Theory and Computation, 2021, 17, 2409-2416.	2.3	16
5	Electrostatic correlations in electrolytes: Contribution of screening ion interactions to the excess chemical potential. Journal of Chemical Physics, 2021, 155, 221102.	1.2	8
6	Recruiting RyRs to Open in a Ca ²⁺ Release Unit: Single-RyR Gating Properties Make RyR Group Dynamics. Biophysical Journal, 2020, 118, 232-242.	0.2	4
7	Modeling the Device Behavior of Biological and Synthetic Nanopores with Reduced Models. Entropy, 2020, 22, 1259.	1.1	7
8	Simulating diffusion from a cluster of point sources using propagation integrals. European Biophysics Journal, 2020, 49, 385-393.	1.2	5
9	Electric Double Layers with Surface Charge Regulation Using Density Functional Theory. Entropy, 2020, 22, 132.	1.1	9
10	Scaling Behavior of Bipolar Nanopore Rectification with Multivalent Ions. Journal of Physical Chemistry C, 2019, 123, 28985-28996.	1.5	20
11	Energetics of counterion adsorption in the electrical double layer. Journal of Chemical Physics, 2019, 150, 154706.	1.2	24
12	Multiscale analysis of the effect of surface charge pattern on a nanopore's rectification and selectivity properties: From all-atom model to Poisson-Nernst-Planck. Journal of Chemical Physics, 2019, 150, 144703.	1.2	26
13	The binding interactions that maintain excitation-contraction coupling junctions in skeletal muscle. Journal of General Physiology, 2019, 151, 593-605.	0.9	8
14	A systematic Monte Carlo simulation study of the primitive model planar electrical double layer over an extended range of concentrations, electrode charges, cation diameters and valences. AIP Advances, 2018, 8, .	0.6	25
15	Sarcoplasmic Reticulum Ca ²⁺ Release Uses a Cascading Network of Intra-SR and Channel Countercurrents. Biophysical Journal, 2018, 114, 462-473.	0.2	22
16	An Experimental Approach to Systematically Probe Charge Inversion in Nanofluidic Channels. Nano Letters, 2018, 18, 1191-1195.	4.5	21
17	Ryanodine Receptor Open Times Are Determined in the Closed State. Biophysical Journal, 2018, 115, 1160-1165.	0.2	12
18	Assessing the accuracy of three classical density functional theories of the electrical double layer. Physical Review E, 2018, 98, 012116.	0.8	26

#	ARTICLE	IF	CITATIONS
19	Sarcoplasmic reticulum Ca ²⁺ , Mg ²⁺ , K ⁺ , and Cl ⁻ concentrations adjust quickly as heart rate changes. <i>Journal of Molecular and Cellular Cardiology</i> , 2017, 103, 31-39.	0.9	9
20	Calsequestrin depolymerizes when calcium is depleted in the sarcoplasmic reticulum of working muscle. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E638-E647.	3.3	55
21	Two-Dimensional Electric Double Layer Structure with Heterogeneous Surface Charge. <i>Langmuir</i> , 2017, 33, 5642-5651.	1.6	9
22	Multiscale modeling of a rectifying bipolar nanopore: explicit-water versus implicit-water simulations. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 17816-17826.	1.3	23
23	Shells of charge: a density functional theory for charged hard spheres. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 244006.	0.7	40
24	(Almost) Stationary Isotachophoretic Concentration Boundary in a Nanofluidic Channel Using Charge Inversion. <i>Analytical Chemistry</i> , 2016, 88, 6145-6150.	3.2	14
25	Improving charge-sensitive biomolecule sensors with the right choice of electrolyte. <i>Sensors and Actuators B: Chemical</i> , 2016, 230, 281-288.	4.0	4
26	PACO: PArticle COunting Method To Enforce Concentrations in Dynamic Simulations. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 925-929.	2.3	9
27	A review of steric interactions of ions: Why some theories succeed and others fail to account for ion size. <i>Microfluidics and Nanofluidics</i> , 2015, 18, 717-738.	1.0	73
28	Algorithm for the Time-Propagation of the Radial Diffusion Equation Based on a Gaussian Quadrature. <i>PLoS ONE</i> , 2015, 10, e0132273.	1.1	3
29	Restoring the consistency with the contact density theorem of a classical density functional theory of ions at a planar electrical double layer. <i>Physical Review E</i> , 2014, 90, 052134.	0.8	8
30	Selective transport through a model calcium channel studied by Local Equilibrium Monte Carlo simulations coupled to the Nernst-Planck equation. <i>Journal of Molecular Liquids</i> , 2014, 189, 100-112.	2.3	23
31	Selecting Ions by Size in a Calcium Channel: The Ryanodine Receptor Case Study. <i>Biophysical Journal</i> , 2014, 107, 2263-2273.	0.2	27
32	Domain and Interdomain Energetics Underlying Gating in Shaker -Type K ⁺ Channels. <i>Biophysical Journal</i> , 2014, 107, 1841-1852.	0.2	9
33	Three-Dimensional Brownian Dynamics Simulator for the Study of Ion Permeation through Membrane Pores. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2911-2926.	2.3	33
34	Dynamic Monte Carlo Simulation of Coupled Transport through a Narrow Multiply-Occupied Pore. <i>Journal of Physical Chemistry C</i> , 2014, 118, 700-707.	1.5	9
35	Sarcoplasmic Reticulum K ⁺ (TRIC) Channel Does Not Carry Essential Countercurrent during Ca ²⁺ Release. <i>Biophysical Journal</i> , 2013, 105, 1151-1160.	0.2	22
36	Pernicious attrition and inter-RyR2 CICR current control in cardiac muscle. <i>Journal of Molecular and Cellular Cardiology</i> , 2013, 58, 53-58.	0.9	50

#	ARTICLE	IF	CITATIONS
37	Computing the partition function, ensemble averages, and density of states for lattice spin systems by sampling the mean. <i>Journal of Computational Physics</i> , 2013, 250, 1-12.	1.9	1
38	Ion Correlations in Nanofluidic Channels: Effects of Ion Size, Valence, and Concentration on Voltage- and Pressure-Driven Currents. <i>Langmuir</i> , 2013, 29, 1303-1317.	1.6	50
39	Separation of Ions in Nanofluidic Channels with Combined Pressure-Driven and Electro-Osmotic Flow. <i>Analytical Chemistry</i> , 2013, 85, 2991-2998.	3.2	48
40	The role of solvation in the binding selectivity of the L-type calcium channel. <i>Journal of Chemical Physics</i> , 2013, 139, 055103.	1.2	24
41	Comparison of three-dimensional Poisson solution methods for particle-based simulation and inhomogeneous dielectrics. <i>Physical Review E</i> , 2012, 86, 011912.	0.8	22
42	Ryanodine Receptor Current Amplitude Controls Ca ²⁺ Sparks in Cardiac Muscle. <i>Circulation Research</i> , 2012, 111, 28-36.	2.0	57
43	High Energy Conversion Efficiency in Nanofluidic Channels. <i>Nano Letters</i> , 2012, 12, 1410-1416.	4.5	111
44	Steady-State Electrodifffusion from the Nernst-Planck Equation Coupled to Local Equilibrium Monte Carlo Simulations. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 824-829.	2.3	43
45	Current and selectivity in a model sodium channel under physiological conditions: Dynamic Monte Carlo simulations. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2012, 1818, 592-600.	1.4	33
46	Modeling Ca ²⁺ Induced Ca ²⁺ Release Between Neighboring Ryanodine Receptors. <i>Biophysical Journal</i> , 2012, 102, 138a.	0.2	1
47	Is ryanodine receptor a calcium or magnesium channel? Roles of K ⁺ and Mg ²⁺ during Ca ²⁺ release. <i>Cell Calcium</i> , 2012, 51, 427-433.	1.1	27
48	Particle-based simulation of charge transport in discrete-charge nano-scale systems: the electrostatic problem. <i>Nanoscale Research Letters</i> , 2012, 7, 135.	3.1	1
49	Particle-based simulation of electrical transport in discrete-charge nanoscale systems: The electrostatic problem. , 2011, , .		0
50	Toward making the mean spherical approximation of primitive model electrolytes analytic: An analytic approximation of the MSA screening parameter. <i>Journal of Chemical Physics</i> , 2011, 134, 044103.	1.2	4
51	Free-Energy Density Functional of Ions at a Dielectric Interface. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 1178-1182.	2.1	12
52	Selectivity sequences in a model calcium channel: role of electrostatic field strength. <i>European Biophysics Journal</i> , 2011, 40, 775-782.	1.2	26
53	Efficiently accounting for ion correlations in electrokinetic nanofluidic devices using density functional theory. <i>Journal of Colloid and Interface Science</i> , 2011, 359, 520-529.	5.0	45
54	Analyzing the components of the free-energy landscape in a calcium selective ion channel by Widom's particle insertion method. <i>Journal of Chemical Physics</i> , 2011, 134, 055102.	1.2	37

#	ARTICLE	IF	CITATIONS
55	A method for treating the passage of a charged hard sphere ion as it passes through a sharp dielectric boundary. <i>Journal of Chemical Physics</i> , 2011, 135, 064105.	1.2	17
56	Sieving experiments and pore diameter: it's not a simple relationship. <i>European Biophysics Journal</i> , 2010, 39, 1513-1521.	1.2	13
57	Selecting Ions by Size in a Calcium Channel: the Ryanodine Receptor Case Study. <i>Biophysical Journal</i> , 2010, 98, 332a.	0.2	6
58	Analytic Theory for Dilute Colloids in a Charged Slit. <i>Journal of Physical Chemistry B</i> , 2010, 114, 4302-4309.	1.2	11
59	Simulations of calcium channel block by trivalent cations: Gd ³⁺ competes with permeant ions for the selectivity filter. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2010, 1798, 2013-2021.	1.4	31
60	An efficient algorithm for classical density functional theory in three dimensions: Ionic solutions. <i>Journal of Chemical Physics</i> , 2010, 132, 124101.	1.2	61
61	Discretization of the induced-charge boundary integral equation. <i>Physical Review E</i> , 2009, 80, 011906.	0.8	24
62	Ionic selectivity in L-type calcium channels by electrostatics and hard-core repulsion. <i>Journal of General Physiology</i> , 2009, 133, 497-509.	0.9	76
63	Protein structure and ionic selectivity in calcium channels: Selectivity filter size, not shape, matters. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2009, 1788, 2471-2480.	1.4	42
64	Ions and Inhibitors in the Binding Site of HIV Protease: Comparison of Monte Carlo Simulations and the Linearized Poisson-Boltzmann Theory. <i>Biophysical Journal</i> , 2009, 96, 1293-1306.	0.2	15
65	Reinterpreting the Anomalous Mole Fraction Effect: The Ryanodine Receptor Case Study. <i>Biophysical Journal</i> , 2009, 97, 2212-2221.	0.2	55
66	Tuning Transport Properties of Nanofluidic Devices with Local Charge Inversion. <i>Journal of the American Chemical Society</i> , 2009, 131, 5194-5202.	6.6	246
67	Energetics of Divalent Selectivity in a Calcium Channel: The Ryanodine Receptor Case Study. <i>Biophysical Journal</i> , 2008, 94, 1169-1184.	0.2	143
68	Bubbles, Gating, and Anesthetics in Ion Channels. <i>Biophysical Journal</i> , 2008, 94, 4282-4298.	0.2	82
69	Volume Exclusion in Calcium Selective Channels. <i>Biophysical Journal</i> , 2008, 94, 3486-3496.	0.2	58
70	The Anomalous Mole Fraction Effect in Calcium Channels: A Measure of Preferential Selectivity. <i>Biophysical Journal</i> , 2008, 95, 2658-2672.	0.2	71
71	Synthetic Nanopores as a Test Case for Ion Channel Theories: The Anomalous Mole Fraction Effect without Single Filing. <i>Biophysical Journal</i> , 2008, 95, 609-619.	0.2	72
72	Intracellular Calcium Release Channels Mediate Their Own Countercurrent: The Ryanodine Receptor Case Study. <i>Biophysical Journal</i> , 2008, 95, 3706-3714.	0.2	99

#	ARTICLE	IF	CITATIONS
73	Simulating prescribed particle densities in the grand canonical ensemble using iterative algorithms. <i>Journal of Chemical Physics</i> , 2008, 128, 124102.	1.2	45
74	Singular perturbation analysis of the steady-state Poisson-Nernst-Planck system: Applications to ion channels. <i>European Journal of Applied Mathematics</i> , 2008, 19, 541-560.	1.4	89
75	Combined Effect of Pore Radius and Protein Dielectric Coefficient on the Selectivity of a Calcium Channel. <i>Physical Review Letters</i> , 2007, 98, 168102.	2.9	78
76	Selective Adsorption of Ions with Different Diameter and Valence at Highly Charged Interfaces. <i>Journal of Physical Chemistry C</i> , 2007, 111, 15575-15585.	1.5	89
77	Steric Selectivity in Na Channels Arising from Protein Polarization and Mobile Side Chains. <i>Biophysical Journal</i> , 2007, 93, 1960-1980.	0.2	111
78	The effect of protein dielectric coefficient on the ionic selectivity of a calcium channel. <i>Journal of Chemical Physics</i> , 2006, 125, 034901.	1.2	93
79	Two Rings of Negative Charges in the Cytosolic Vestibule of Type-1 Ryanodine Receptor Modulate Ion Fluxes. <i>Biophysical Journal</i> , 2006, 90, 443-453.	0.2	65
80	Ca ²⁺ Selectivity of a Chemically Modified OmpF with Reduced Pore Volume. <i>Biophysical Journal</i> , 2006, 91, 4392-4400.	0.2	49
81	Density functional theory of the electrical double layer: the RFD functional. <i>Journal of Physics Condensed Matter</i> , 2005, 17, 6609-6626.	0.7	94
82	Physics of Size Selectivity. <i>Physical Review Letters</i> , 2005, 95, 247801.	2.9	56
83	(De)constructing the Ryanodine Receptor: Modeling Ion Permeation and Selectivity of the Calcium Release Channel. <i>Journal of Physical Chemistry B</i> , 2005, 109, 15598-15610.	1.2	121
84	Probing the Role of Negatively Charged Amino Acid Residues in Ion Permeation of Skeletal Muscle Ryanodine Receptor. <i>Biophysical Journal</i> , 2005, 89, 256-265.	0.2	66
85	Monte Carlo simulation of the electric double layer: dielectric boundaries and the effects of induced charge. <i>Molecular Physics</i> , 2005, 103, 2851-2861.	0.8	29
86	Computing induced charges in inhomogeneous dielectric media: Application in a Monte Carlo simulation of complex ionic systems. <i>Physical Review E</i> , 2004, 69, 046702.	0.8	138
87	Monte Carlo Simulation Study of a System with a Dielectric Boundary: Application to Calcium Channel Selectivity. <i>Molecular Simulation</i> , 2004, 30, 89-96.	0.9	35
88	Permeation Properties of an Engineered Bacterial OmpF Porin Containing the EEEE-Locus of Ca ²⁺ Channels. <i>Biophysical Journal</i> , 2004, 87, 3137-3147.	0.2	77
89	Relating Microscopic Charge Movement to Macroscopic Currents: The Ramo-Shockley Theorem Applied to Ion Channels. <i>Biophysical Journal</i> , 2004, 87, 3716-3722.	0.2	36
90	Density functional theory of charged, hard-sphere fluids. <i>Physical Review E</i> , 2003, 68, 031503.	0.8	159

#	ARTICLE	IF	CITATIONS
91	Coupling Poisson-Nernst-Planck and density functional theory to calculate ion flux. Journal of Physics Condensed Matter, 2002, 14, 12129-12145.	0.7	238
92	A physical mechanism for large-ion selectivity of ion channels. Physical Chemistry Chemical Physics, 2002, 4, 4763-4769.	1.3	32
93	Physical descriptions of experimental selectivity measurements in ion channels. European Biophysics Journal, 2002, 31, 454-466.	1.2	78
94	Ion Accumulation in a Biological Calcium Channel: Effects of Solvent and Confining Pressure. Journal of Physical Chemistry B, 2001, 105, 6427-6436.	1.2	97