Dirk Gillespie

List of Publications by Year
in descending order

94 papers	4,208 citations	81900 39 h-index	114465 63 g-index
96 all docs	96 docs citations	96 times ranked	2419 citing authors

#	Article	IF	Citations
1	Tuning Transport Properties of Nanofluidic Devices with Local Charge Inversion. Journal of the American Chemical Society, 2009, 131, 5194-5202.	13.7	246
2	Coupling PoissonÂNernstÂPlanck and density functional theory to calculate ion flux. Journal of Physics Condensed Matter, 2002, 14, 12129-12145.	1.8	238
3	Density functional theory of charged, hard-sphere fluids. Physical Review E, 2003, 68, 031503.	2.1	159
4	Energetics of Divalent Selectivity in a Calcium Channel: The Ryanodine Receptor Case Study. Biophysical Journal, 2008, 94, 1169-1184.	0.5	143
5	Computing induced charges in inhomogeneous dielectric media: Application in a Monte Carlo simulation of complex ionic systems. Physical Review E, 2004, 69, 046702.	2.1	138
6	(De)constructing the Ryanodine Receptor:Â Modeling Ion Permeation and Selectivity of the Calcium Release Channel. Journal of Physical Chemistry B, 2005, 109, 15598-15610.	2.6	121
7	Steric Selectivity in Na Channels Arising from Protein Polarization and Mobile Side Chains. Biophysical Journal, 2007, 93, 1960-1980.	0.5	111
8	High Energy Conversion Efficiency in Nanofluidic Channels. Nano Letters, 2012, 12, 1410-1416.	9.1	111
9	Intracellular Calcium Release Channels Mediate Their Own Countercurrent: The Ryanodine Receptor Case Study. Biophysical Journal, 2008, 95, 3706-3714.	0.5	99
10	Ion Accumulation in a Biological Calcium Channel:Â Effects of Solvent and Confining Pressure. Journal of Physical Chemistry B, 2001, 105, 6427-6436.	2.6	97
11	Density functional theory of the electrical double layer: the RFD functional. Journal of Physics Condensed Matter, 2005, 17, 6609-6626.	1.8	94
12	The effect of protein dielectric coefficient on the ionic selectivity of a calcium channel. Journal of Chemical Physics, 2006, 125, 034901.	3.0	93
13	Selective Adsorption of Ions with Different Diameter and Valence at Highly Charged Interfaces. Journal of Physical Chemistry C, 2007, 111, 15575-15585.	3.1	89
14	Singular perturbation analysis of the steady-state Poissonâ€“Nernstâ€“Planck system: Applications to ion channels. European Journal of Applied Mathematics, 2008, 19, 541-560.	2.9	89
15	Bubbles, Gating, and Anesthetics in Ion Channels. Biophysical Journal, 2008, 94, 4282-4298.	0.5	82
16	Physical descriptions of experimental selectivity measurements in ion channels. European Biophysics Journal, 2002, 31, 454-466.	2.2	78
17	Combined Effect of Pore Radius and Protein Dielectric Coefficient on the Selectivity of a Calcium Channel. Physical Review Letters, 2007, 98, 168102.	7.8	78
18	Permeation Properties of an Engineered Bacterial OmpF Porin Containing the EEEE-Locus of Ca2+ Channels. Biophysical Journal, 2004, 87, 3137-3147.	0.5	77

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19	Ionic selectivity in L-type calcium channels by electrostatics and hard-core repulsion. Journal of General Physiology, 2009, 133, 497-509.	1.9	76
20	A review of steric interactions of ions: Why some theories succeed and others fail to account for ion size. Microfluidics and Nanofluidics, 2015, 18, 717-738.	2.2	73
21	Synthetic Nanopores as a Test Case for Ion Channel Theories: The Anomalous Mole Fraction Effect without Single Filing. Biophysical Journal, 2008, 95, 609-619.	0.5	72
22	The Anomalous Mole Fraction Effect in Calcium Channels: A Measure of Preferential Selectivity. Biophysical Journal, 2008, 95, 2658-2672.	0.5	71
23	Probing the Role of Negatively Charged Amino Acid Residues in Ion Permeation of Skeletal Muscle Ryanodine Receptor. Biophysical Journal, 2005, 89, 256-265.	0.5	66
24	Two Rings of Negative Charges in the Cytosolic Vestibule of Type-1 Ryanodine Receptor Modulate Ion Fluxes. Biophysical Journal, 2006, 90, 443-453.	0.5	65
25	An efficient algorithm for classical density functional theory in three dimensions: Ionic solutions. Journal of Chemical Physics, 2010, 132, 124101.	3.0	61
26	Volume Exclusion in Calcium Selective Channels. Biophysical Journal, 2008, 94, 3486-3496.	0.5	58
27	Ryanodine Receptor Current Amplitude Controls Ca ²⁺ Sparks in Cardiac Muscle. Circulation Research, 2012, 111, 28-36.	4.5	57
28	Physics of Size Selectivity. Physical Review Letters, 2005, 95, 247801.	7.8	56
29	Reinterpreting the Anomalous Mole Fraction Effect: The Ryanodine Receptor Case Study. Biophysical Journal, 2009, 97, 2212-2221.	0.5	55
30	Calsequestrin depolymerizes when calcium is depleted in the sarcoplasmic reticulum of working muscle. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E638-E647.	7.1	55
31	Pernicious attrition and inter-RyR2 CICR current control in cardiac muscle. Journal of Molecular and Cellular Cardiology, 2013, 58, 53-58.	1.9	50
32	Ion Correlations in Nanofluidic Channels: Effects of Ion Size, Valence, and Concentration on Voltage- and Pressure-Driven Currents. Langmuir, 2013, 29, 1303-1317.	3.5	50
33	Ca2+ Selectivity of a Chemically Modified OmpF with Reduced Pore Volume. Biophysical Journal, 2006, 91, 4392-4400.	0.5	49
34	Separation of Ions in Nanofluidic Channels with Combined Pressure-Driven and Electro-Osmotic Flow. Analytical Chemistry, 2013, 85, 2991-2998.	6.5	48
35	Simulating prescribed particle densities in the grand canonical ensemble using iterative algorithms. Journal of Chemical Physics, 2008, 128, 124102.	3.0	45
36	Efficiently accounting for ion correlations in electrokinetic nanofluidic devices using density functional theory. Journal of Colloid and Interface Science, 2011, 359, 520-529.	9.4	45

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37	Steady-State Electrodiffusion from the Nernstâ€“Planck Equation Coupled to Local Equilibrium Monte Carlo Simulations. Journal of Chemical Theory and Computation, 2012, 8, 824-829.	5.3	43
38	Protein structure and ionic selectivity in calcium channels: Selectivity filter size, not shape, matters. Biochimica Et Biophysica Acta - Biomembranes, 2009, 1788, 2471-2480.	2.6	42
39	Shells of charge: a density functional theory for charged hard spheres. Journal of Physics Condensed Matter, 2016, 28, 244006.	1.8	40
40	Analyzing the components of the free-energy landscape in a calcium selective ion channel by Widom's particle insertion method. Journal of Chemical Physics, 2011, 134, 055102.	3.0	37
41	Relating Microscopic Charge Movement to Macroscopic Currents: The Ramo-Shockley Theorem Applied to Ion Channels. Biophysical Journal, 2004, 87, 3716-3722.	0.5	36
42	Monte Carlo Simulation Study of a System with a Dielectric Boundary: Application to Calcium Channel Selectivity. Molecular Simulation, 2004, 30, 89-96.	2.0	35
43	Current and selectivity in a model sodium channel under physiological conditions: Dynamic Monte Carlo simulations. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 592-600.	2.6	33
44	Three-Dimensional Brownian Dynamics Simulator for the Study of Ion Permeation through Membrane Pores. Journal of Chemical Theory and Computation, 2014, 10, 2911-2926.	5.3	33
45	A physical mechanism for large-ion selectivity of ion channels. Physical Chemistry Chemical Physics, 2002, 4, 4763-4769.	2.8	32
46	Simulations of calcium channel block by trivalent cations: Gd3+ competes with permeant ions for the selectivity filter. Biochimica Et Biophysica Acta - Biomembranes, 2010, 1798, 2013-2021.	2.6	31
47	Monte Carlo simulation of the electric double layer: dielectric boundaries and the effects of induced charge. Molecular Physics, 2005, 103, 2851-2861.	1.7	29
48	Is ryanodine receptor a calcium or magnesium channel? Roles of K+ and Mg2+ during Ca2+ release. Cell Calcium, 2012, 51, 427-433.	2.4	27
49	Selecting Ions by Size in a Calcium Channel: The Ryanodine Receptor Case Study. Biophysical Journal, 2014, 107, 2263-2273.	0.5	27
50	Selectivity sequences in a model calcium channel: role of electrostatic field strength. European Biophysics Journal, 2011, 40, 775-782.	2.2	26
51	Assessing the accuracy of three classical density functional theories of the electrical double layer. Physical Review E, 2018, 98, 012116.	2.1	26
52	Multiscale analysis of the effect of surface charge pattern on a nanoporeâ€™s rectification and selectivity properties: From all-atom model to Poisson-Nernst-Planck. Journal of Chemical Physics, 2019, 150, 144703.	3.0	26
53	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, .	1.3	25
54	Discretization of the induced-charge boundary integral equation. Physical Review E, 2009, 80, 011906.	2.1	24

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55	The role of solvation in the binding selectivity of the L-type calcium channel. Journal of Chemical Physics, 2013, 139, 055103.	3.0	24
56	Energetics of counterion adsorption in the electrical double layer. Journal of Chemical Physics, 2019, 150, 154706.	3.0	24
57	Selective transport through a model calcium channel studied by Local Equilibrium Monte Carlo simulations coupled to the Nernstâ€“Planck equation. Journal of Molecular Liquids, 2014, 189, 100-112.	4.9	23
58	Multiscale modeling of a rectifying bipolar nanopore: explicit-water versus implicit-water simulations. Physical Chemistry Chemical Physics, 2017, 19, 17816-17826.	2.8	23
59	Comparison of three-dimensional Poisson solution methods for particle-based simulation and inhomogeneous dielectrics. Physical Review E, 2012, 86, 011912.	2.1	22
60	Sarcoplasmic Reticulum K+ (TRIC) Channel Does Not Carry Essential Countercurrent during Ca2+ Release. Biophysical Journal, 2013, 105, 1151-1160.	0.5	22
61	Sarcoplasmic Reticulum Ca2+ Release Uses aÂCascading Network of Intra-SR and Channel Countercurrents. Biophysical Journal, 2018, 114, 462-473.	0.5	22
62	An Experimental Approach to Systematically Probe Charge Inversion in Nanofluidic Channels. Nano Letters, 2018, 18, 1191-1195.	9.1	21
63	Scaling Behavior of Bipolar Nanopore Rectification with Multivalent Ions. Journal of Physical Chemistry C, 2019, 123, 28985-28996.	3.1	20
64	A method for treating the passage of a charged hard sphere ion as it passes through a sharp dielectric boundary. Journal of Chemical Physics, 2011, 135, 064105.	3.0	17
65	Revisiting the Charged Shell Model: A Density Functional Theory for Electrolytes. Journal of Chemical Theory and Computation, 2021, 17, 2409-2416.	5.3	16
66	Ions and Inhibitors in the Binding Site of HIV Protease: Comparison ofÂMonte Carlo Simulations and the Linearized Poisson-Boltzmann Theory. Biophysical Journal, 2009, 96, 1293-1306.	0.5	15
67	(Almost) Stationary Isotachophoretic Concentration Boundary in a Nanofluidic Channel Using Charge Inversion. Analytical Chemistry, 2016, 88, 6145-6150.	6.5	14
68	Sieving experiments and pore diameter: itâ€™s not a simple relationship. European Biophysics Journal, 2010, 39, 1513-1521.	2.2	13
69	Free-Energy Density Functional of Ions at a Dielectric Interface. Journal of Physical Chemistry Letters, 2011, 2, 1178-1182.	4.6	12
70	Ryanodine Receptor Open Times Are Determined in the Closed State. Biophysical Journal, 2018, 115, 1160-1165.	0.5	12
71	Analytic Theory for Dilute Colloids in a Charged Slit. Journal of Physical Chemistry B, 2010, 114, 4302-4309.	2.6	11
72	Domain and Interdomain Energetics Underlying Gating in Shaker -Type K V Channels. Biophysical Journal, 2014, 107, 1841-1852.	0.5	9

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73	Dynamic Monte Carlo Simulation of Coupled Transport through a Narrow Multiply-Occupied Pore. Journal of Physical Chemistry C, 2014, 118, 700-707.	3.1	9
74	PACO: PArticle COunting Method To Enforce Concentrations in Dynamic Simulations. Journal of Chemical Theory and Computation, 2016, 12, 925-929.	5.3	9
75	Sarcoplasmic reticulum Ca 2+ , Mg 2+ , K + , and Cl â^' concentrations adjust quickly as heart rate changes. Journal of Molecular and Cellular Cardiology, 2017, 103, 31-39.	1.9	9
76	Two-Dimensional Electric Double Layer Structure with Heterogeneous Surface Charge. Langmuir, 2017, 33, 5642-5651.	3.5	9
77	Electric Double Layers with Surface Charge Regulation Using Density Functional Theory. Entropy, 2020, 22, 132.	2.2	9
78	Restoring the consistency with the contact density theorem of a classical density functional theory of ions at a planar electrical double layer. Physical Review E, 2014, 90, 052134.	2.1	8
79	The binding interactions that maintain excitationâ€“contraction coupling junctions in skeletal muscle. Journal of General Physiology, 2019, 151, 593-605.	1.9	8
80	Electrostatic correlations in electrolytes: Contribution of screening ion interactions to the excess chemical potential. Journal of Chemical Physics, 2021, 155, 221102.	3.0	8
81	Modeling the Device Behavior of Biological and Synthetic Nanopores with Reduced Models. Entropy, 2020, 22, 1259.	2.2	7
82	Selecting Ions by Size in a Calcium Channel: the Ryanodine Receptor Case Study. Biophysical Journal, 2010, 98, 332a.	0.5	6
83	Individual ion species chemical potentials in the Mean Spherical Approximation. Journal of Chemical Physics, 2022, 156, .	3.0	6
84	Simulating diffusion from a cluster of point sources using propagation integrals. European Biophysics Journal, 2020, 49, 385-393.	2.2	5
85	Simulating cardiac Ca2+ release units: effects of RyR cluster size and Ca2+ buffers on diastolic Ca2+ leak. Pflugers Archiv European Journal of Physiology, 2021, 473, 435-446.	2.8	5
86	Toward making the mean spherical approximation of primitive model electrolytes analytic: An analytic approximation of the MSA screening parameter. Journal of Chemical Physics, 2011, 134, 044103.	3.0	4
87	Improving charge-sensitive biomolecule sensors with the right choice of electrolyte. Sensors and Actuators B: Chemical, 2016, 230, 281-288.	7.8	4
88	Recruiting RyRs to Open in a Ca2+ Release Unit: Single-RyR Gating Properties Make RyR Group Dynamics. Biophysical Journal, 2020, 118, 232-242.	0.5	4
89	Algorithm for the Time-Propagation of the Radial Diffusion Equation Based on a Gaussian Quadrature. PLoS ONE, 2015, 10, e0132273.	2.5	3
90	Physical interpretation of theories of homogeneous electrolytes in the primitive model. Journal of Molecular Liquids, 2022, 362, 119785.	4.9	3

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91	Modeling Ca2+ Induced Ca2+ Release Between Neighboring Ryanodine Receptors. Biophysical Journal, 2012, 102, 138a.	0.5	1
92	Particle-based simulation of charge transport in discrete-charge nano-scale systems: the electrostatic problem. Nanoscale Research Letters, 2012, 7, 135.	5.7	1
93	Computing the partition function, ensemble averages, and density of states for lattice spin systems by sampling the mean. Journal of Computational Physics, 2013, 250, 1-12.	3.8	1
94	Particle-based simulation of electrical transport in discrete-charge nanoscale systems: The electrostatic problem. , 2011, , .		0