# Dirk Gillespie

List of Publications by Year
in descending order



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|---|---|---|---|
| 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 | Individual ion species chemical potentials in the Mean Spherical Approximation. Journal of Chemical Physics, 2022, 156, . | 3.0 | 6 |
| 2 | Physical interpretation of theories of homogeneous electrolytes in the primitive model. Journal of Molecular Liquids, 2022, 362, 119785. | 4.9 | 3 |
| 3 | 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 |
| 4 | Revisiting the Charged Shell Model: A Density Functional Theory for Electrolytes. Journal of Chemical Theory and Computation, 2021, 17, 2409-2416. | 5.3 | 16 |
| 5 | Electrostatic correlations in electrolytes: Contribution of screening ion interactions to the excess chemical potential. Journal of Chemical Physics, 2021, 155, 221102. | 3.0 | 8 |
| 6 | 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 |
| 7 | Modeling the Device Behavior of Biological and Synthetic Nanopores with Reduced Models. Entropy, 2020, 22, 1259. | 2.2 | 7 |
| 8 | Simulating diffusion from a cluster of point sources using propagation integrals. European Biophysics Journal, 2020, 49, 385-393. | 2.2 | 5 |
| 9 | Electric Double Layers with Surface Charge Regulation Using Density Functional Theory. Entropy, 2020, 22, 132. | 2.2 | 9 |
| 10 | Scaling Behavior of Bipolar Nanopore Rectification with Multivalent Ions. Journal of Physical Chemistry C, 2019, 123, 28985-28996. | 3.1 | 20 |
| 11 | Energetics of counterion adsorption in the electrical double layer. Journal of Chemical Physics, 2019, 150, 154706. | 3.0 | 24 |
| 12 | 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 |
| 13 | The binding interactions that maintain excitationâ€“contraction coupling junctions in skeletal muscle. Journal of General Physiology, 2019, 151, 593-605. | 1.9 | 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, . | 1.3 | 25 |
| 15 | Sarcoplasmic Reticulum Ca2+ Release Uses aÂCascading Network of Intra-SR and Channel Countercurrents. Biophysical Journal, 2018, 114, 462-473. | 0.5 | 22 |
| 16 | An Experimental Approach to Systematically Probe Charge Inversion in Nanofluidic Channels. Nano Letters, 2018, 18, 1191-1195. | 9.1 | 21 |
| 17 | Ryanodine Receptor Open Times Are Determined in the Closed State. Biophysical Journal, 2018, 115, 1160-1165. | 0.5 | 12 |
| 18 | Assessing the accuracy of three classical density functional theories of the electrical double layer. Physical Review E, 2018, 98, 012116. | 2.1 | 26 |

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|---|---|---|---|
| 19 | 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 |
| 20 | 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 |
| 21 | Two-Dimensional Electric Double Layer Structure with Heterogeneous Surface Charge. Langmuir, 2017, 33, 5642-5651. | 3.5 | 9 |
| 22 | Multiscale modeling of a rectifying bipolar nanopore: explicit-water versus implicit-water simulations. Physical Chemistry Chemical Physics, 2017, 19, 17816-17826. | 2.8 | 23 |
| 23 | Shells of charge: a density functional theory for charged hard spheres. Journal of Physics Condensed Matter, 2016, 28, 244006. | 1.8 | 40 |
| 24 | (Almost) Stationary Isotachophoretic Concentration Boundary in a Nanofluidic Channel Using Charge Inversion. Analytical Chemistry, 2016, 88, 6145-6150. | 6.5 | 14 |
| 25 | Improving charge-sensitive biomolecule sensors with the right choice of electrolyte. Sensors and Actuators B: Chemical, 2016, 230, 281-288. | 7.8 | 4 |
| 26 | PACO: PArticle COunting Method To Enforce Concentrations in Dynamic Simulations. Journal of Chemical Theory and Computation, 2016, 12, 925-929. | 5.3 | 9 |
| 27 | 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 |
| 28 | Algorithm for the Time-Propagation of the Radial Diffusion Equation Based on a Gaussian Quadrature. PLoS ONE, 2015, 10, e0132273. | 2.5 | 3 |
| 29 | 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 |
| 30 | 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 |
| 31 | Selecting Ions by Size in a Calcium Channel: The Ryanodine Receptor Case Study. Biophysical Journal, 2014, 107, 2263-2273. | 0.5 | 27 |
| 32 | Domain and Interdomain Energetics Underlying Gating in Shaker -Type K V Channels. Biophysical Journal, 2014, 107, 1841-1852. | 0.5 | 9 |
| 33 | 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 |
| 34 | 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 |
| 35 | Sarcoplasmic Reticulum K+ (TRIC) Channel Does Not Carry Essential Countercurrent during Ca2+ Release. Biophysical Journal, 2013, 105, 1151-1160. | 0.5 | 22 |
| 36 | Pernicious attrition and inter-RyR2 CICR current control in cardiac muscle. Journal of Molecular and Cellular Cardiology, 2013, 58, 53-58. | 1.9 | 50 |

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|---|---|---|---|
| 37 | 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 |
| 38 | 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 |
| 39 | Separation of Ions in Nanofluidic Channels with Combined Pressure-Driven and Electro-Osmotic Flow. Analytical Chemistry, 2013, 85, 2991-2998. | 6.5 | 48 |
| 40 | The role of solvation in the binding selectivity of the L-type calcium channel. Journal of Chemical Physics, 2013, 139, 055103. | 3.0 | 24 |
| 41 | Comparison of three-dimensional Poisson solution methods for particle-based simulation and inhomogeneous dielectrics. Physical Review E, 2012, 86, 011912. | 2.1 | 22 |
| 42 | Ryanodine Receptor Current Amplitude Controls Ca <sup>2+</sup> Sparks in Cardiac Muscle. Circulation Research, 2012, 111, 28-36. | 4.5 | 57 |
| 43 | High Energy Conversion Efficiency in Nanofluidic Channels. Nano Letters, 2012, 12, 1410-1416. | 9.1 | 111 |
| 44 | 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 |
| 45 | 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 |
| 46 | Modeling Ca2+ Induced Ca2+ Release Between Neighboring Ryanodine Receptors. Biophysical Journal, 2012, 102, 138a. | 0.5 | 1 |
| 47 | 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 |
| 48 | Particle-based simulation of charge transport in discrete-charge nano-scale systems: the electrostatic problem. Nanoscale Research Letters, 2012, 7, 135. | 5.7 | 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. Journal of Chemical Physics, 2011, 134, 044103. | 3.0 | 4 |
| 51 | Free-Energy Density Functional of Ions at a Dielectric Interface. Journal of Physical Chemistry Letters, 2011, 2, 1178-1182. | 4.6 | 12 |
| 52 | Selectivity sequences in a model calcium channel: role of electrostatic field strength. European Biophysics Journal, 2011, 40, 775-782. | 2.2 | 26 |
| 53 | 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 |
| 54 | 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 |

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|---|---|---|---|
| 55 | 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 |
| 56 | Sieving experiments and pore diameter: itâ€™s not a simple relationship. European Biophysics Journal, 2010, 39, 1513-1521. | 2.2 | 13 |
| 57 | Selecting Ions by Size in a Calcium Channel: the Ryanodine Receptor Case Study. Biophysical Journal, 2010, 98, 332a. | 0.5 | 6 |
| 58 | Analytic Theory for Dilute Colloids in a Charged Slit. Journal of Physical Chemistry B, 2010, 114, 4302-4309. | 2.6 | 11 |
| 59 | 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 |
| 60 | An efficient algorithm for classical density functional theory in three dimensions: Ionic solutions. Journal of Chemical Physics, 2010, 132, 124101. | 3.0 | 61 |
| 61 | Discretization of the induced-charge boundary integral equation. Physical Review E, 2009, 80, 011906. | 2.1 | 24 |
| 62 | Ionic selectivity in L-type calcium channels by electrostatics and hard-core repulsion. Journal of General Physiology, 2009, 133, 497-509. | 1.9 | 76 |
| 63 | 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 |
| 64 | 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 |
| 65 | Reinterpreting the Anomalous Mole Fraction Effect: The Ryanodine Receptor Case Study. Biophysical Journal, 2009, 97, 2212-2221. | 0.5 | 55 |
| 66 | Tuning Transport Properties of Nanofluidic Devices with Local Charge Inversion. Journal of the American Chemical Society, 2009, 131, 5194-5202. | 13.7 | 246 |
| 67 | Energetics of Divalent Selectivity in a Calcium Channel: The Ryanodine Receptor Case Study. Biophysical Journal, 2008, 94, 1169-1184. | 0.5 | 143 |
| 68 | Bubbles, Gating, and Anesthetics in Ion Channels. Biophysical Journal, 2008, 94, 4282-4298. | 0.5 | 82 |
| 69 | Volume Exclusion in Calcium Selective Channels. Biophysical Journal, 2008, 94, 3486-3496. | 0.5 | 58 |
| 70 | The Anomalous Mole Fraction Effect in Calcium Channels: A Measure of Preferential Selectivity. Biophysical Journal, 2008, 95, 2658-2672. | 0.5 | 71 |
| 71 | 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 |
| 72 | Intracellular Calcium Release Channels Mediate Their Own Countercurrent: The Ryanodine Receptor Case Study. Biophysical Journal, 2008, 95, 3706-3714. | 0.5 | 99 |

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|---|---|---|---|
| 73 | Simulating prescribed particle densities in the grand canonical ensemble using iterative algorithms. Journal of Chemical Physics, 2008, 128, 124102. | 3.0 | 45 |
| 74 | 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 |
| 75 | 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 |
| 76 | 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 |
| 77 | Steric Selectivity in Na Channels Arising from Protein Polarization and Mobile Side Chains. Biophysical Journal, 2007, 93, 1960-1980. | 0.5 | 111 |
| 78 | The effect of protein dielectric coefficient on the ionic selectivity of a calcium channel. Journal of Chemical Physics, 2006, 125, 034901. | 3.0 | 93 |
| 79 | 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 |
| 80 | Ca2+ Selectivity of a Chemically Modified OmpF with Reduced Pore Volume. Biophysical Journal, 2006, 91, 4392-4400. | 0.5 | 49 |
| 81 | Density functional theory of the electrical double layer: the RFD functional. Journal of Physics Condensed Matter, 2005, 17, 6609-6626. | 1.8 | 94 |
| 82 | Physics of Size Selectivity. Physical Review Letters, 2005, 95, 247801. | 7.8 | 56 |
| 83 | (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 |
| 84 | 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 |
| 85 | 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 |
| 86 | 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 |
| 87 | 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 |
| 88 | Permeation Properties of an Engineered Bacterial OmpF Porin Containing the EEEE-Locus of Ca2+ Channels. Biophysical Journal, 2004, 87, 3137-3147. | 0.5 | 77 |
| 89 | Relating Microscopic Charge Movement to Macroscopic Currents: The Ramo-Shockley Theorem Applied to Ion Channels. Biophysical Journal, 2004, 87, 3716-3722. | 0.5 | 36 |
| 90 | Density functional theory of charged, hard-sphere fluids. Physical Review E, 2003, 68, 031503. | 2.1 | 159 |

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|---|---|---|---|
| 91 | Coupling PoissonÂNernstÂPlanck and density functional theory to calculate ion flux. Journal of Physics Condensed Matter, 2002, 14, 12129-12145. | 1.8 | 238 |
| 92 | A physical mechanism for large-ion selectivity of ion channels. Physical Chemistry Chemical Physics, 2002, 4, 4763-4769. | 2.8 | 32 |
| 93 | Physical descriptions of experimental selectivity measurements in ion channels. European Biophysics Journal, 2002, 31, 454-466. | 2.2 | 78 |
| 94 | 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 |