

# DIRK GILLESPIE

## PERSONAL INFORMATION

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Department of Physiology and Biophysics  
Rush University Medical Center  
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Born in (West) Germany in 1972  
Citizenship: Germany  
Visa status: U.S. permanent resident

## ACADEMIC POSITIONS

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Rush University Medical Center  
*Professor* (2022 – present)  
*Associate Professor* (2011 – 2022)  
*Assistant Professor* (2003 – 2011)

University of Miami School of Medicine  
*Voluntary Assistant Professor* (2003 – 2005)  
*Non-Enrolled (Postdoctoral) Fellow* (2000 – 2003)

University of Texas at Austin  
*Lecturer* (January 2000 – May 2000)  
*Visiting Scholar* (October 1999 – January 2000)

Rush University (Rush-Presbyterian-St. Luke's Medical Center)  
*Visiting Instructor* (1999 – 2003)  
*Instructor* (1998 – 1999)

## EDUCATION

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Rush University, Chicago, IL (1996 – 1999)  
*Ph.D. in Physiology/Biophysics*

Northwestern University, Evanston, IL (1994 – 1996)  
*M.Sc. in Mathematics*

Johns Hopkins University, Baltimore, MD (1990 – 1994)  
*B.A. in Mathematics*

## PEER-REVIEWED PUBLICATIONS

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### ► most significant papers

1. N. Salles Vernin, E. do Amaral Soares, F. Tavares and D. Gillespie, Charge inversion in 1:1 electrolytes: Analyzing the energetics, *Journal of Physical Chemistry B* 127, 4318-4327 (2023).
2. N. Salles Vernin and D. Gillespie, Surface charge regulation using classical density functional theory: the effect of divalent potential determining ions, *Physical Chemistry Chemical Physics* 25, 1023-1031 (2022).
3. R.J. Tomlin, T. Roy, T.L. Kirk, M. Marinescu and D. Gillespie, Impedance response of ionic liquids in long slit pores, *Journal of the Electrochemical Society* 169, 120513 (2022).
4. ► D. Gillespie, Numerical solution of compartment-based reaction/diffusion models with DABOSS algorithm, *European Biophysics Journal* 51, 595–607 (2022).
5. H. Fábíán, Z. Sarkadi, M. Valiskó, D. Gillespie and D. Boda, Calcium versus potassium selectivity in a nanopore: The effect of charge inversion at localized pore charges, *Journal of Molecular Liquids* 368, 120715 (2022).
6. D. Gillespie, Physical interpretation of theories of homogeneous electrolytes in the primitive model, *Journal of Molecular Liquids* 362, 119785 (2022).
7. ► J.S. Høye and D. Gillespie, Individual ion species chemical potentials in the Mean Spherical Approximation, *Journal of Chemical Physics* 156, 244110 (2022).
8. ► D. Gillespie, M. Valiskó and D. Boda, Electrostatic correlations in electrolytes: Contribution of screening ion interactions to the excess chemical potential, *Journal of Chemical Physics* 155, 221102 (2021).
9. J. Jiang and D. Gillespie, Revisiting the charged shell model: a density functional theory for electrolytes, *Journal of Chemical Theory and Computation* 17, 2409–2416 (2021).
10. M. Fill and D. Gillespie, Simulating cardiac  $\text{Ca}^{2+}$  release units: Effects of RyR cluster size and  $\text{Ca}^{2+}$  buffers on diastolic  $\text{Ca}^{2+}$  leak, *Pfluegers Archiv* 473, 435-446 (2021).
11. D. Boda, M. Valiskó and D. Gillespie, Modeling the device behavior of biological and synthetic nanopores with reduced models, *Entropy* 22, 1259 (2020).
12. ► D. Gillespie, Simulating diffusion from a cluster of point sources using propagation integrals, *European Biophysics Journal* 49, 385-293 (2020).
13. D. Gillespie, D.N. Petsev and F. von Swol, Electric double layers with surface charge regulation using density functional theory, *Entropy* 22, 132 (2020).
14. ► D. Gillespie, Recruiting RyRs to open in a  $\text{Ca}^{2+}$  release unit: Single-RyR gating properties make RyR group dynamics, *Biophysical Journal* 118, 232-242 (2020).
15. D. Fertig, B. Matejczyk, M. Valiskó, D. Gillespie and D. Boda, Scaling behavior of bipolar nanopore rectification with multivalent ions, *Journal of Physical Chemistry C* 123, 28985-28996 (2019).
16. ► A. Voukadinova and D. Gillespie, Energetics of counterion adsorption in the electrical double layer, *Journal of Chemical Physics* 150, 154706 (2019). **Editor's Choice Selection**
17. M. Valiskó, B. Matejczyk, Z. Ható, T. Kristóf, E. Má dai, D. Fertig, D. Gillespie and D. Boda, 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* 150, 144703 (2019).

18. E. Ríos, D. Gillespie and C. Franzini-Armstrong, The binding interactions that maintain excitation–contraction coupling junctions in skeletal muscle, *Journal of General Physiology* 151, 593-605 (2019).
19. ► M. Fill and D. Gillespie, Ryanodine receptor open times are determined in the closed state, *Biophysical Journal* 115, 1160-1165 (2018).
20. A. Voukadinova, M. Valiskó and D. Gillespie, Assessing the accuracy of three classical density functional theories of the electrical double layer, *Physical Review E* 98, 012116 (2018).
21. M. Valiskó, T. Kristóf, D. Gillespie and D. Boda, 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* 8, 025320 (2018).
22. ► K.-H. Chou, C. McCallum, D. Gillespie and S. Pennathur, An experimental approach to systematically probe charge inversion in nanofluidic channels, *Nano Letters* 18, 1191-1195 (2018).
23. ► V. Zsolnay, M. Fill and D. Gillespie, Sarcoplasmic reticulum  $\text{Ca}^{2+}$  release uses a cascading network of intra-SR and channel countercurrents, *Biophysical Journal* 114, 462-473 (2018).
24. Z. Ható, M. Valiskó, T. Kristóf, D. Gillespie and D. Boda, Multiscale modeling of a rectifying bipolar nanopore: Explicit-water versus implicit-water simulations, *Physical Chemistry Chemical Physics* 19, 17816-17826 (2017).
25. ► C. McCallum, S. Pennathur and D. Gillespie, Two-dimensional electric double layer structure with heterogeneous surface charge, *Langmuir* 33, 5642-5651 (2017).
26. C. Manno, L. Figueroa, D. Gillespie, R. Fitts, C. Kang, C. Franzini-Armstrong and E. Ríos, 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* 114, E638-E647 (2017).
27. C. Berti, V. Zsolnay, T.R. Shannon, M. Fill and D. Gillespie, Sarcoplasmic reticulum  $\text{Ca}^{2+}$ ,  $\text{Mg}^{2+}$ ,  $\text{K}^+$ , and  $\text{Cl}^-$  concentrations adjust quickly as heart rate changes, *Journal of Molecular and Cellular Cardiology* 103, 31-39 (2017).
28. ► J. Loessberg-Zahl, K.G.H. Janssen, C. McCallum, D. Gillespie and S. Pennathur, (Almost) stationary isotachophoretic concentration boundary in a nanofluidic channel using charge inversion, *Analytical Chemistry* 88, 6145-6150 (2016).
29. ► R. Roth and D. Gillespie, Shells of charge: A density functional theory for charged hard spheres, *Journal of Physics: Condensed Matter* 28, 244006 (2016).
30. L. Friedrich and D. Gillespie, Improving charge-sensitive biomolecule sensors with the right choice of electrolyte, *Sensors and Actuators B: Chemical* 230, 281-288 (2016).
31. ► C. Berti, S. Furini and D. Gillespie, PACO: PArticle COunting method to enforce concentrations in dynamic simulations, *Journal of Chemical Theory and Computation* 12, 925-929 (2016).
32. Z. Ható, D. Boda, D. Gillespie, J. Vrabec, G. Rutkai and T. Kristóf, Simulation study of a rectifying bipolar ion channel: Detailed model versus reduced model, *Condensed Matter Physics* 19, 13802 (2016).
33. D. Gillespie, Algorithm for the time-propagation of the radial diffusion equation based on a Gaussian quadrature, *PLoS ONE* 10, e0132273 (2015).

34. ► D. Gillespie, A review of steric interactions of ions: Why some theories succeed and others fail to account for ion size, *Microfluidics and Nanofluidics* 18, 717-738 (2015). **Invited Review**
35. D. Gillespie, 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* 90, 052134 (2014).
36. ► D. Gillespie, L. Xu and G. Meissner, Selecting ions by size in a calcium channel: The ryanodine receptor case study, *Biophysical Journal* 107, 2263-2273 (2014). *selected for Best of 2014 issue of Biophysical Journal*
37. A. Peyser, D. Gillespie, R. Roth and W. Nonner, Domain and interdomain energetics underlying gating in *Shaker*-type K<sub>v</sub> channels, *Biophysical Journal* 107, 1841-1852 (2014).
38. ► D. Boda, É. Csányi, D. Gillespie and T. Kristóf, Dynamic Monte Carlo simulation of coupled transport through a narrow multiply-occupied pore, *Journal of Chemical Physics* 118, 700-707 (2014).
39. C. Berti, S. Furini, D. Gillespie, D. Boda, R.S. Eisenberg, E. Sangiorgi and C. Fiegna, Three-dimensional Brownian dynamics simulator for the study of ion permeation through membrane pores, *Journal of Chemical Theory and Computation* 10, 2911-2926 (2014).
40. D. Boda, R. Kovács, D. Gillespie and T. Kristóf, Selective transport through a model calcium channel studied by Local Equilibrium Monte Carlo simulations coupled to the Nernst-Planck equation, *Journal of Molecular Liquids* 189, 100-112 (2014).
41. D. Boda, D. Henderson and D. Gillespie, The role of solvation in the binding selectivity of the L-type calcium channel, *Journal of Chemical Physics* 139, 055103 (2013).
42. ► T. Guo, A. Nani, S. Shonts, M. Perryman, H. Chen, T.R. Shannon, D. Gillespie and M. Fill, Sarcoplasmic reticulum K<sup>+</sup> (TRIC) channel does not carry essential countercurrent during Ca<sup>2+</sup> release, *Biophysical Journal* 105, 1151-1160 (2013).
43. D. Gillespie, Computing the partition function, ensemble averages, and density of states for lattice spin systems by sampling the mean, *Journal of Computational Physics* 250, 1-12 (2013).
44. D. Gillespie and S. Pennathur, Separation of ions in nanofluidic channels with combined pressure-driven and electro-osmotic flow, *Analytical Chemistry* 85, 2991-2998 (2013).
45. ► D. Gillespie and M. Fill, Pernicious attrition and inter-RyR2 CICR current control in cardiac muscle, *Journal of Molecular and Cellular Cardiology* 58, 53-58 (2013). **Invited Review**
46. ► J. Hoffmann and D. Gillespie, Ion correlations in nanofluidic channels: Effects of ion size, valence, and concentration on voltage- and pressure-driven currents, *Langmuir* 29, 1303-1317 (2013).
47. C. Berti, D. Gillespie, J.P. Bardhan, R.S. Eisenberg and C. Fiegna, Comparison of three-dimensional Poisson solution methods for particle-based simulation and inhomogeneous dielectrics, *Physical Review E* 86, 011912 (2012).
48. ► T. Guo, D. Gillespie and M. Fill, Ryanodine receptor current amplitude controls Ca<sup>2+</sup> sparks in cardiac muscle, *Circulation Research* 111, 28-36 (2012).
49. ► D. Gillespie, High energy conversion efficiency in nanofluidic channels, *Nano Letters* 12, 1410-1416 (2012).

50. ► D. Gillespie, H. Chen and M. Fill, Is ryanodine receptor a calcium or magnesium channel? Roles of  $K^+$  and  $Mg^{2+}$  during  $Ca^{2+}$  release, *Cell Calcium* 51, 427-433 (2012).
51. C. Berti, D. Gillespie, R.S. Eisenberg and C. Fiegna, Particle-based simulation of charge transport in discrete-charge nanoscale systems: The electrostatic problem, *Nanoscale Research Letters* 7, 135 (2012).
52. ► D. Boda and D. Gillespie, Steady-state electrodiffusion from the Nernst-Planck equation coupled to local equilibrium Monte Carlo simulations, *Journal of Chemical Theory and Computation* 8, 824-829 (2012).
53. É. Csányi, D. Boda, D. Gillespie and T. Kristóf, Current and selectivity in a model sodium channel under physiological conditions: Dynamic Monte Carlo simulations, *Biochimica et Biophysica Acta (BBA) - Biomembranes* 1818, 592-600 (2012).
54. D. Boda, D. Henderson, R.S. Eisenberg and D. Gillespie, A method for treating the passage of a charged hard sphere ion as it passes through a sharp dielectric boundary, *Journal of Chemical Physics* 135, 064105 (2011).
55. ► D. Gillespie, Free-energy density functional of ions at a dielectric interface, *Journal of Physical Chemistry Letters* 2, 1178-1182 (2011).
56. ► D. Gillespie, A.S. Khair, J.P. Bardhan and S. Pennathur, Efficiently accounting for ion correlations in electrokinetic nanofluidic devices using density functional theory, *Journal of Colloid and Interface Science* 359, 520-529 (2011).
57. ► D. Krauss, B. Eisenberg and D. Gillespie, Selectivity sequences in a model calcium channel: Role of electrostatic field strength, *European Biophysics Journal* 40, 775-782 (2011).
58. D. Boda, J. Giri, D. Henderson, B. Eisenberg and D. Gillespie, Analyzing the components of the free energy landscape in a calcium selective ion channel by Widom's particle insertion method, *Journal of Chemical Physics* 134, 055102 (2011). *selected for JCP website **Research Highlights***
59. D. Gillespie, Toward making the mean spherical approximation of primitive model electrolytes analytic: An analytic approximation of the MSA screening parameter, *Journal of Chemical Physics* 134, 044103 (2011).
60. A. Malasics, D. Boda, M. Valiskó, D. Henderson and D. Gillespie, Simulations of calcium channel block by trivalent cations:  $Gd^{3+}$  competes with permeant ions for the selectivity filter, *Biochimica et Biophysica Acta (BBA) - Biomembranes* 1798, 2013-2021 (2010).
61. D. Krauss and D. Gillespie, Sieving experiments and pore diameter: It's not a simple relationship, *European Biophysics Journal* 39, 1513-1521 (2010).
62. D. Gillespie, Analytic theory for dilute colloids in a charged slit, *Journal of Physical Chemistry B* 114, 4302-4309 (2010).
63. ► M.G. Knepley, D. Karpeev, S. Davidovits, R.S. Eisenberg and D. Gillespie, An efficient algorithm for classical density functional theory in three dimensions: Ionic solutions, *Journal of Chemical Physics* 132, 124101 (2010).
64. A. Malasics, D. Gillespie, W. Nonner, D. Henderson, B. Eisenberg and D. Boda, Protein structure and ionic selectivity in calcium channels: Selectivity filter size, not shape, matters, *Biochimica et Biophysica Acta (BBA) - Biomembranes* 1788, 2471-2480 (2009).
65. ► D. Gillespie, J. Giri and M. Fill, Reinterpreting the anomalous mole fraction effect: The ryanodine receptor case study, *Biophysical Journal* 97, 2212-2221 (2009).

66. J.P. Bardhan, R.S. Eisenberg and D. Gillespie, Discretization of the induced-charge boundary integral equation, *Physical Review E* 80, 011906 (2009).
67. ► D. Boda, M. Valiskó, D. Henderson, B. Eisenberg, D. Gillespie and W. Nonner, Ionic selectivity in L-type calcium channels by electrostatics and hard-core repulsion, *Journal of General Physiology* 133, 497-509 (2009).
68. ► Y. He, D. Gillespie, D. Boda, I. Vlassiuk, R.S. Eisenberg and Z.S. Siwy, Tuning transport properties of nanofluidic devices with local charge inversion, *Journal of the American Chemical Society* 131, 5194-5202 (2009).
69. D. Boda, M. Valiskó, D. Henderson, D. Gillespie, B. Eisenberg and M.K. Gilson, Ions and inhibitors in the binding site of HIV-protease: Comparison of Monte Carlo simulations and the linearized Poisson-Boltzmann theory, *Biophysical Journal* 96, 1293-1306 (2009).
70. ► D. Gillespie and M. Fill, Intracellular calcium release channels mediate their own countercurrent: The ryanodine receptor case study, *Biophysical Journal* 95, 3706-3714 (2008).
71. ► D. Gillespie and D. Boda, The anomalous mole fraction effect in calcium channels: A measure of preferential selectivity, *Biophysical Journal* 95, 2658-2672 (2008).
72. A. Singer, D. Gillespie, J. Norbury and R.S. Eisenberg, Singular perturbation analysis of the steady state Poisson-Nernst-Planck system: Applications to ion channels, *European Journal of Applied Mathematics* 19, 541-560 (2008).
73. ► D. Gillespie, D. Boda, Y. He, P. Apel and Z.S. Siwy, Synthetic nanopores as a test case for ion channel theories: The anomalous mole fraction effect without single filing, *Biophysical Journal* 95, 609-619 (2008).
74. ► R. Roth, D. Gillespie, W. Nonner and R.E. Eisenberg, Bubbles, gating, and anesthetics in ion channels, *Biophysical Journal* 94, 4282-4298 (2008).
75. A. Malasics, D. Gillespie and D. Boda, Simulating prescribed particle densities in the grand canonical ensemble using iterative algorithms, *Journal of Chemical Physics* 128, 124102 (2008).
76. D. Boda, W. Nonner, D. Henderson, B. Eisenberg and D. Gillespie, Volume exclusion in calcium selective channels, *Biophysical Journal* 94, 3486-3496 (2008).
77. ► D. Gillespie, Energetics of divalent selectivity in a calcium channel: The ryanodine receptor case study, *Biophysical Journal* 94, 1169-1184 (2008).
78. M. Valiskó, D. Boda and D. Gillespie, Selective adsorption of ions with different diameter and valence at highly-charged interfaces, *Journal of Physical Chemistry C* 111, 15575-15585 (2007).
79. D. Boda, W. Nonner, M. Valiskó, D. Henderson, B. Eisenberg and D. Gillespie, Steric selectivity in Na channels arising from protein polarization and mobile side chains, *Biophysical Journal* 93, 1960-1980 (2007).
80. ► D. Boda, M. Valiskó, B. Eisenberg, W. Nonner, D. Henderson and D. Gillespie, Combined effect of pore radius and protein dielectric coefficient on the selectivity of a calcium channel, *Physical Review Letters* 98, 168102 (2007).
81. H. Miedema, M. Vrouenraets, J. Wierenga, D. Gillespie, B. Eisenberg, W. Meijberg and W. Nonner, Ca<sup>2+</sup> selectivity of a chemically modified OmpF with reduced pore volume, *Biophysical Journal* 91, 4392-4400 (2006).

82. ► D. Boda, M. Valiskó, B. Eisenberg, W. Nonner, D. Henderson and D. Gillespie, The effect of protein dielectric coefficient on the ionic selectivity of a calcium channel, *Journal of Chemical Physics* 125, 034901 (2006).
83. L. Xu, Y. Wang, D. Gillespie and G. Meissner, Two rings of negative charges in the cytosolic vestibule of type-1 ryanodine receptor modulate ion fluxes, *Biophysical Journal* 90, 443-453 (2006).
84. R. Roth and D. Gillespie, Physics of size selectivity, *Physical Review Letters* 95, 247801 (2005).
85. ► D. Gillespie, M. Valiskó and D. Boda, Density functional theory of the electrical double layer: the RFD functional, *Journal of Physics: Condensed Matter* 17, 6609-6626 (2005).
86. D. Henderson, D. Gillespie, T. Nagy and D. Boda, Monte Carlo simulation of the electric double layer: dielectric boundaries and the effects of induced charge, *Molecular Physics* 103, 2851-2861 (2005).
87. ► D. Gillespie, L. Xu, Y. Wang and G. Meissner, (De)constructing the ryanodine receptor: Modeling ion permeation and selectivity of the calcium release channel, *Journal of Physical Chemistry B* 109, 15598-15610 (2005).
88. Y. Wang, L. Xu, D.A. Pasek, D. Gillespie and G. Meissner, Probing the role of negatively charged amino acid residues in ion permeation of skeletal muscle ryanodine receptor, *Biophysical Journal* 89, 256-265 (2005).
89. W. Nonner, A. Peyser, D. Gillespie and B. Eisenberg, Relating microscopic charge movement to macroscopic currents: The Ramo-Shockley theorem applied to ion channels, *Biophysical Journal* 87, 3716-3722 (2004).
90. H. Miedema, A. Meter-Arkema, J. Wierenga, J. Tang, B. Eisenberg, W. Nonner, H. Hektor, D. Gillespie and W. Meijberg, Permeation properties of an engineered bacterial OmpF porin containing the EEEE-Locus of Ca<sup>2+</sup> channels, *Biophysical Journal* 87, 3137-3147 (2004).
91. ► D. Boda, D. Gillespie, W. Nonner, D. Henderson and B. Eisenberg, Computing induced charges in inhomogeneous dielectric media: Application in a Monte Carlo simulation of complex ionic systems, *Physical Review E* 69, 046702 (2004).
92. D. Boda, T. Varga, D. Henderson, D.D. Busath, W. Nonner, D. Gillespie and B. Eisenberg, Monte Carlo simulation study of a system with a dielectric boundary: Application to calcium channel selectivity, *Molecular Simulation* 30, 89-96 (2004).
93. ► D. Gillespie, W. Nonner and R.S. Eisenberg, Density functional theory of charged, hard-sphere fluids, *Physical Review E* 68, 031503 (2003).
94. ► D. Gillespie, W. Nonner and R.S. Eisenberg, Coupling Poisson-Nernst-Planck and density functional theory to calculate ion flux, *Journal of Physics: Condensed Matter* 14, 12129-12145 (2002).
95. ► D. Gillespie and R.S. Eisenberg, Physical descriptions of experimental selectivity measurements in ion channels, *European Biophysics Journal* 31, 454-466 (2002).
96. D. Gillespie, W. Nonner, D. Henderson and R.S. Eisenberg, A physical mechanism for large-ion selectivity in ion channels, *Physical Chemistry Chemical Physics* 4, 4763-4769 (2002).
97. W. Nonner, D. Gillespie, D. Henderson and B. Eisenberg, Ion accumulation in a biological calcium channel: effects of solvent and confining pressure, *Journal of Physical Chemistry B* 105, 6427-6436 (2001).

98. D. Gillespie and R.S. Eisenberg, Modified Donnan potentials for ion transport through biological ion channels, *Physical Review E* 62, 061902 (2001).

#### **NONPEER-REVIEWED PUBLICATIONS**

---

1. D. Boda and D. Gillespie, Calculating the electrostatic potential profiles of double layers from simulation ion density profiles, *Hungarian Journal of Industry and Chemistry* 41, 123-130 (2013).
2. D. Gillespie, Fundamentals of electrostatics, *Protein Folding-Misfolding: Some Current Concepts of Protein Chemistry*, 199 (2007).
3. D. Boda, D. Gillespie, B. Eisenberg, W. Nonner and D. Henderson, Induced charge computation method, *Ionic Soft Matter: Modern Trends in Theory and Applications*, 19-43 (2005).
4. D. Henderson, D. Boda, and D. Gillespie, Computer simulations of ions in inhomogeneous dielectric materials, *Proceedings of the 2004 International Conference on MEMS, NANO and Smart Systems*, 179-180. IEEE Computer Society, IEEE, Los Alamitos, CA (2004).
5. D. Gillespie, W. Nonner, and R. S. Eisenberg, Crowded charge in biological ion channels, *Nanotech 2003 (Proceedings)*, vol. 3, 435-438 (2003).

## INVITED SEMINARS

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Tel-Aviv University, Israel (*Department of Mathematics*)  
Max Planck Institute for Medical Research (Heidelberg) (*Dept. of Cell Physiology*)  
University of Texas Austin (*Department of Mathematics*)  
College of William and Mary (*Department of Applied Science*)  
University of Konstanz, Germany (*Department of Mathematics and Statistics*)  
University of Veszprém, Hungary (*Department of Physical Chemistry*)  
Max Planck Institute for Metals Research, Stuttgart, Germany  
University of Utrecht, The Netherlands (*Department of Physics*)  
Heinrich Heine University, Germany (*Department of Physics*)  
Carnegie-Mellon University (*Department of Chemistry*)  
Oxford University, England (*Department of Mathematics*)  
University of Illinois, Urbana-Champaign (*Department of Material Science*)  
University of California, Irvine (*Department of Physics and Astronomy*)  
University of North Carolina, Chapel Hill (*Dept. of Biochemistry & Biophysics*)  
Sandia National Laboratory  
University of California, Santa Barbara (*Molecular, Cell, Developmental Biology*)  
University of Wisconsin, Milwaukee (*Department of Mathematical Sciences*)  
University of Pannonia, Hungary (*Departments of Physics & Physical Chemistry*)  
Slovak Academy of Sciences (*Institute of Molecular Physiology and Genetics*)  
University of Erlangen, Germany (*Department of Theoretical Physics I*)  
University of Maryland (*Institute for Physical Science and Technology*)  
University of Bologna, Cesna, Italy  
Virginia Commonwealth University (*Department of Physiology and Biophysics*)  
University of Chicago (*Institute of Integrative Physiology*)  
University of Washington (*Department of Materials Science and Engineering*)  
Stanford University (*Department of Mechanical Engineering*)  
University of Twente, The Netherlands (*Institute for Nanotechnology*)  
Ohio State University (*Mathematical Biosciences Institute*)  
University of California, San Diego (*Center for Theoretical Biological Physics*)  
University of Michigan (*Center for Arrhythmia Research*)  
Arizona State University (*Department of Physics*)  
University of Illinois at Chicago (*Department of Bioengineering*)  
University of Dundee, Scotland (*Life Sciences*)  
University of Glasgow (*Institute of Cardiovascular and Medical Sciences*)  
Aix-Marseille University, France (*Bio-AFM Lab*)  
University of New Mexico (*Department of Chemical and Biological Engineering*)  
Oxford University, England (*Biochemistry*)  
Oxford University, England (*Pharmacology*)  
Federal University of Rio de Janeiro (*Applied Thermodynamics and Simulation*)

## **INVITED CONFERENCE/WORKSHOP TALKS**

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Biophysical Society, Permeation/Transport Subgroup meeting 2006  
Gordon Conference, Ion Channels 2006  
Ionic Transport: from Nanopores to Biological Channels 2007 (*Lyon, France*)  
Johann Radon Institute for Computational & Applied Mathematics (*Linz, Austria*)  
Society for Industrial & Applied Mathematics Conf. on Dynamical Systems 2007  
Ion Channel Biophysics Workshop 2007 (*Telluride, CO*)  
American Chemical Society, Northwest & Rocky Mountain Regional Mtg. 2008  
Society for Industrial and Applied Mathematics Annual Meeting 2009  
Gordon Conference, Muscle: Excitation/Contraction Coupling 2009 (poster highlight)  
Ion Channel Biophysics Workshop 2009 (*Telluride, CO*)  
Mathematical Biosciences Institute workshop on “Modeling and Computation of Biomolecular Structure and Dynamics” 2011 (*Ohio State University*)  
International Congress on Industrial and Applied Mathematics 2011 (*Vancouver*)  
Ion Channel Biophysics Workshop 2011 (*Telluride, CO*)  
Workshop on Mathematical Modeling of Ion Channels 2011 (*Oxford University*)  
Gordon Conference, Muscle: Excitation/Contraction Coupling 2012 (poster highlight)  
Joint Meeting of the Hungarian Anatomical, Biophysical, Microcirculation, and Vascular Biology Societies 2012 (*Debrecen, Hungary*)  
Ion Channel Biophysics Workshop 2013 (*Telluride, CO*)  
Tübingen Density Functional Days Workshop 2013 (*Tübingen, Germany*)  
Condensed Matter Physics Symposium 2014 (*Brigham Young University*)  
Tübingen Density Functional Days Workshop 2014 (*Tübingen, Germany*)  
Gordon Conference, Muscle: Excitation/Contraction Coupling 2015 (poster highlight)  
Ion Channel Biophysics Workshop 2015 (*Telluride, CO*)  
Tübingen Density Functional Days Workshop 2015 (*Tübingen, Germany*)  
Rush Research Forum 2016 (*Rush University, Chicago*)  
Soft Matter at Interfaces Workshop 2017 (*Max Planck Society, Germany*)  
Ion Channel Biophysics Workshop 2017 (*Telluride, CO*)  
Tübingen Density Functional Days Workshop 2017 (*Tübingen, Germany*)  
American Physical Society March Meeting 2018  
Ion Channel Biophysics Workshop 2019 (*Telluride, CO*)  
Tübingen Density Functional Days Workshop 2019 (*Tübingen, Germany*)  
Tübingen Density Functional Days Workshop 2020 (*virtual*)  
Ion Channel Biophysics Workshop 2021 (*Telluride, CO*)  
Tübingen Density Functional Days Workshop 2021 (*virtual*)

## HONORS

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- University of Pannonia (Hungary)  
winner *Pannonia Award* (2020). Given to foreign scientists who contributed to the international recognition of the University through long term scientific collaborations and establishing new fields and scopes of research at the University
- Rush University Medical Center  
winner *University Committee on Research Grant* (2005)
- Society for Industrial and Applied Mathematics (SIAM)  
winner *SIAM Student Paper Prize* (1999)
- Rush University  
*Carlson Luckhardt Endowed Scholarship* for academic excellence (1998)
- Johns Hopkins University  
*Department of Mathematics Honors* (1994)  
*General Honors* (1994)  
*William S. Todman Scholarship* for academic excellence (1992 and 1993)

## TEACHING EXPERIENCE

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- Rush University Medical Center, Dept. of Molecular Biophysics and Physiology  
*Associate Course Director* for Physiology 502 (formerly 452), the second of the two-quarter physiology course for first-year medical students.  
2006 – 2010.  
*lecturer* in Physiology, acid/base balance, fluid balance, temperature regulation.  
2006 – 2017.
- University of Miami School of Medicine, Department of Physiology & Biophysics  
*taught* Basic Mathematical and Computational Methods for Scientists in Fall 2002.  
Personally proposed, designed, and taught the class
- University of Texas at Austin, Department of Mathematics  
*taught Matrices and Matrix Calculations* Spring 2000 (100+ students)
- Northwestern University, Department of Mathematics  
*teaching assistant* for various levels of Calculus, Linear Algebra, Real Analysis, and Complex Analysis (1994 – 1996). Duties included one hour per week sessions for lecturing and answering questions; writing and grading quizzes; grading exams; holding office hours; lecturing when professor was absent.

## PROFESSIONAL MEMBERSHIPS

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- Biophysical Society  
*member* (1996 – present)  
*Chair*, Permeation and Transport Subgroup (2012 – 2014)  
*Vice Chair*, Permeation and Transport Subgroup (2010 – 2012)  
*Secretary/Treasurer*, Permeation and Transport Subgroup (2008 – 2010)
- American Chemical Society  
*member* (2010 – present)

## **EDITING AND REVIEWING**

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*European Biophysics Journal* (published by Springer)

Handling Editor (2016 – present)

Advisory Editor (2009 – 2016)

*Channels* (published by Landes Biosciences)

Editorial Board (2013 – present)

*PLOS Computational Biology* (published by Public Library of Science)

Guest Editor (2015 – present), multiple manuscripts

*Hungarian Journal of Industry and Chemistry* (published by De Gruyter Open)

Editorial Board (2015 – present)

*Annual Reports in Computational Chemistry* (American Chemical Society)

co-editor of Biological Modeling with Nathan Baker (2012, 2014)

Grant applications reviewed for: U.S. National Science Foundation, German Science Foundation (Deutsche Forschungsgemeinschaft), Netherlands Organisation for Scientific Research (NWO), Research Grants Council of Hong Kong, University of California System, Swiss National Science Foundation, Czech Science Foundation

Journal articles reviewed in:

physics, chemistry, technology, and mathematics: *Nature Nanotechnology*, *Nature Communications*, *Physical Review Letters*, *Physical Review E*, *Langmuir*, *Journal of Chemical Physics*, *Journal of Physical Chemistry*, *Journal of Physics: Condensed Matter*, *Advances in Colloid and Interface Science*, *Colloids and Surfaces A*, *SIAM Journal on Applied Mathematics*

biology: *Circulation*, *Biophysical Journal*, *Journal of General Physiology*, *European Biophysics Journal*, *BBA Biomembranes*

## **UNIVERSITY SERVICE**

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University Council (Rush University, Rush University Medical Center)

*member* (2020 – 2024)

Faculty Council (Rush Medical College, Rush University Medical Center)

*Chair* (2021 – 2022)

*Secretary* (2019 – 2020)

*member* (2016 – 2022)

Department Advisory Committee

*member* (2011 – present)

Graduate College Interim Admission Committee (Rush University Medical Center)

*member* (2015)

Graduate College Council (Rush University Medical Center)

*Elected Representative of Division of Molecular Biophysics and Physiology* (2014 – 2016)

Graduate College Re-engineering Committee (Rush University Medical Center)

*member* (2014 – 2017)

Committee on Curriculum and Evaluation (Rush University Medical Center)

*member* (2009 – 2015)

M1 (first-year medical student) Workgroup (Rush University Medical Center)

*member* (2006 – 2015)

Committee for M1 curriculum change (Rush University Medical Center)

*member* (2006 – 2008)

## **STUDENTS AND POSTDOCTORAL FELLOWS SUPERVISED**

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Ruben Tomlin (2020 – present)

*research advisor* (Imperial College, London). Ruben is a postdoc at ICL working on DFT of supercapacitors. I am working with him to implement code and guide his project on an informal basis.

Adelina Voukadinova (2017 – 2018)

*undergraduate student* (University of Illinois at Chicago). Adi analyzed DFT calculations of the electrical double layer and authored two papers [9,13].

Vilmos Zsolnay (2016 – 2017)

*undergraduate student* (Northwestern University). Vil worked on the SR compartment model developed by Claudio Berti, identifying the role of SR  $K^+$  channels. He presented his work in a poster at the 2017 Biophysical Society meeting and authored a paper [16].

Elizabeth Baetz (summer of 2015)

*undergraduate student* (Northwestern University).

Leanne Friedrich (spring and summer of 2015)

*undergraduate student* (Northwestern University). Leanne analyzed how different electrolytes change sensor sensitivity, authoring one paper [23].

Pinar Arikian (spring of 2014)

*undergraduate student* (Northwestern University). Pinar used a “toy” model of calcium channels to understand what properties these channels have under physiological conditions.

Christopher McCallum (2013 – 2017)

*graduate student* (University of California, Santa Barbara). Co-supervisor of his PhD thesis project with Prof. Sumita Pennathur. Chris computed the effects of ion correlations on nanofluidic ion flow. He successfully defended his thesis in May 2017.

Claudio Berti (September 2013 – September 2015)

*postdoc*. Claudio is developing a compartment-based model of how ions cycle in and out of the sarcoplasmic reticulum during a heartbeat.

Garo Sarajian (summer of 2013)

*undergraduate student* (Johns Hopkins University). Garo studied the effectiveness of a sampling algorithm for lattice spin systems I created.

Jeremiah Jones (2013)

*graduate student* (Arizona State University). I was external reader of his PhD thesis.

Michael J. Yonkunas (September 2010 – December 2012)

*postdoc*. Mike modeled calcium-induced calcium release in cardiac muscle. He won (but declined for personal reasons) an American Heart Association postdoctoral fellowship.

Jordan Hoffmann (summers of 2011 and 2012)

*undergraduate student* (Johns Hopkins University). Jordan’s work to compute the effects of ion-ion and ion-wall correlations in nanofluidic devices [39].

Eduardo Mejia (summer of 2011)  
*high school student.*

Daniel Krauss (summers of 2009 and 2010)  
*undergraduate student* (Grinnell College, Iowa). Dan's work with a "toy" model of a calcium channel led to a poster at the 2010 Biophysical Society meeting and two papers [50,54].

## **CURRENT AND RECENT GRANT SUPPORT**

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*Principal Investigator* on National Science Foundation Award 1402897, 2014-2018. Collaborative Research: Electrokinetic transport and separation in MEMS fabricated nanofluidic channels. This project aims to develop new molecular separation techniques using nanofluidic devices.

*co-Investigator* on NIH R01 AR054098 (Michael Fill, PI), 2013-2018. Sarcoplasmic reticulum K channel function. This project aims to understand the cycle of ion movements into and out of the sarcoplasmic reticulum before, during, and after muscle contraction.

*Principal Investigator* on American Heart Association Award 14GRNT20380691, 2014-2016. Anti-arrhythmic action of carvedilol through a RyR-targeted mechanism. This project combines experiments and modeling to understand the antiarrhythmic action of carvedilol and carvedilol-derived drugs.

*co-Investigator* on NIH R01 HL057832 (Michael Fill, PI), 2012-2015. Control Mechanisms of Ca-Induced Ca Release. This project seeks to define mechanisms that control single cardiac ryanodine receptor function and the process of calcium-induced calcium release (CICR), specifically the functional significance of single ryanodine receptor  $\text{Ca}^{2+}$  current amplitude during CICR.

*co-Investigator* on NIH R01 AR054098 (Michael Fill, PI), 2007-2013. Skeletal muscle ryanodine receptor permeation and self counter-ion flow. This project aims to understand whether the ryanodine receptor (RyR) calcium channel mediates the countercurrent of ions needed to sustain calcium release from intracellular stores.

*Principal Investigator* on Army Research Office grant W911NF-09-1-0488, 9/2009-2012. Classical density functional theory of fluids: Ions at a dielectric interface. This is a theory development project to include dielectric interfaces into the density functional theory of fluids. This is a large gap in the DFT that prevents its general applicability to many applications, including ion channels where my co-workers and I have shown the significant impact the dielectric constant of the protein can have on the channel's selectivity properties.

## **REFERENCES**

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Michael Fill, Department of Molecular Biophysics and Physiology, Rush University Medical Center, 1750 West Harrison Street #1255, Chicago, IL 60612. (312) 942-6434. michael\_fill@rush.edu

Lothar Blatter, Department of Molecular Biophysics and Physiology, Rush University Medical Center, 1750 West Harrison Street #1422, Chicago, IL 60612. (312) 563-3238. lothar\_blatter@rush.edu

Sumita Pennathur, Department of Mechanical Engineering, University of California at Santa Barbara, Engineering Science Building (ESB) #2328, Santa Barbara, CA 93106. (805) 893-5510. sumita@engineering.ucsb.edu







