**Crowded Charges Bibliography**

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**Early Papers**

**Predecessor Papers in the context of PNP (not crowded charges, not L type Ca2+ channel)**

Chen, D., L. Xu, A. Tripathy, G. Meissner, and R. Eisenberg, Permeation through the calcium release channel of cardiac muscle*.* Biophys. J., 1997. **73**(3): p. 1337-1354.

Chen, D.P., Nonequilibrium thermodynamics of transports in ion channels, in *Progress of Cell Research: Towards Molecular Biophysics of Ion Channels*, M. Sokabe, A. Auerbach, and F. Sigworth, Editors. 1997, Elsevier, Amsterdam. p. p. 269-277.

Chen, D., L. Xu, A. Tripathy, G. Meissner, and B. Eisenberg, Selectivity and Permeation in Calcium Release Channel of Cardiac Muscle: Alkali Metal Ions*.* Biophysical Journal, 1999. **76**: p. 1346-1366.

Chen, D., L. Xu, B. Eisenberg, and G. Meissner, Calcium Ion Permeation through the Calcium Release Channel (Ryanodine Receptor) of Cardiac Muscle*.* J Physical Chemistry, 2003. **107B**: p. 9139-9145.

Chen, D.P., W. Nonner, and R.S. Eisenberg, PNP theory fits current-voltage (IV) relations of a neuronal anion channel in 13 solutions. Biophys. J., 1995. **68**: p. A370.

Nonner, W., D.P. Chen, and B. Eisenberg, Anomalous Mole Fraction Effect, Electrostatics, and Binding in Ionic Channels*.* Biophysical Journal, 1998. **74**: p. 2327-2334.

**Early Papers on L type Ca2+ channel, with idea of crowded charges.**

**Abstracts and brief paper documenting first work came from Nonner and Eisenberg**

Catacuzzeno, L., W. Nonner, L. Blum, and B. Eisenberg, Ca Selectivity in the 'EEEE' Locus of L-type Ca Channels*.* Biophysical Journal, 1999. **76**: p. A259.

Nonner, W., D.P. Chen, and B. Eisenberg, Progress and Prospects in Permeation*.* Journal of General Physiology, 1999. **113** (June): p. 773-782.

Nonner, W., L. Catacuzzeno, and B. Eisenberg, Ionic selectivity in calcium channels*.* Biophysical Journal, 2000. **78**: p. A455. (Abstract)

**First crowded charge papers**

Nonner, W. and B. Eisenberg, Ion Permeation and Glutamate Residues Linked by Poisson-Nernst-Planck Theory in L-type Calcium Channels*.* Biophys. J., 1998. **75**: p. 1287-1305.

Nonner, W., L. Catacuzzeno, and B. Eisenberg, Binding and Selectivity in L-type Ca Channels: a Mean Spherical Approximation*.* Biophysical Journal, 2000. **79**: p. 1976-1992.

**Monte Carlo Papers to Check Crude Theories (idea: Henderson; coding Boda)**

Boda, D., D.D. Busath, D. Henderson, and S. Sokolowski, Monte Carlo Simulations of the Mechanism of Channel Selectivity: the competition between Volume Exclusion and Charge Neutrality*.* Journal of Physical Chemistry B, 2000. ***104***: p. 8903-8910.

Boda, D., D. Henderson, and D.D. Busath, Monte Carlo Study of the Effect of Ion and Channel Size on the Selectivity of a Model Calcium Channel*.* Journal of Physical Chemistry B, 2001. **105**(47): p. 11574-11577.

**Subsequent collaborative work with Henderson, Gillespie, and Boda in various combinations**

Nonner, W., D. Gillespie, D. Henderson, and B. Eisenberg, Ion accumulation in a biological calcium channel: effects of solvent and confining pressure*.* J Physical Chemistry B, 2001. **105**: p. 6427-6436.

Boda, D., D. Busath, B. Eisenberg, D. Henderson, and W. Nonner, Monte Carlo simulations of ion selectivity in a biological Na+ channel: charge-space competition*.* Physical Chemistry Chemical Physics (PCCP), 2002. **4**: p. 5154-5160.

Boda, D., D. Busath, B. Eisenberg, D. Henderson, and W. Nonner, Monte Carlo simulations of ion selectivity in a biological Na+ channel: charge-space competition*.* Physical Chemistry Chemical Physics (PCCP), 2002. **4**: p. 5154-5160.

Gillespie, D., W. Nonner, and R.S. Eisenberg, Coupling Poisson-Nernst-Planck and Density Functional Theory to Calculate Ion Flux*.* Journal of Physics (Condensed Matter), 2002. **14**: p. 12129-12145.

Gillespie, D., W. Nonner, and R.S. Eisenberg, Physical model of selectivity and flux in Na channels*.* Biophysical Journal Abstract, 2002. **84**: p. 67a.

Gillespie, D., W. Nonner, D. Henderson, and R.S. Eisenberg, A physical mechanism for large-ion selectivity of ion channels*.* Physical Chemistry Chemical Physics, 2002. **4**: p. 4763-4769.

Gillespie, D., W. Nonner, and R.S. Eisenberg, Density functional theory of charged, hard-sphere fluids. Physical Review E, 2003. **68**: p. 0313503.

Boda, D., 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*.* Phys Rev E Stat Nonlin Soft Matter Phys, 2004. **69**(4 Pt 2): p. 046702.

Boda, D., T. Varga, D. Henderson, 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 2004. **30**: p. 89-96.

Miedema, H., 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 Ca2+ channels*.* Biophys J, 2004. **87**(5): p. 3137-47.

Nonner, W., A. Peyser, D. Gillespie, and B. Eisenberg, Relating microscopic charge movement to macroscopic currents: the Ramo-Shockley theorem applied to ion channels*.* Biophys J, 2004. **87**(6): p. 3716-22.

Boda, D., M. Valisko, B. Eisenberg, W. Nonner, D. Henderson, and D. Gillespie, Effect of Protein Dielectric Coefficient on the Ionic Selectivity of a Calcium Channel*.* Journal of Chemical Physics 2006. **125**: p. 034901.

Miedema, H., M. Vrouenraets, J. Wierenga, B. Eisenberg, D. Gillespie, W. Meijberg, and W. Nonner, Ca2+ selectivity of a chemically modified OmpF with reduced pore volume*.* Biophysical Journal, 2006. **91**: p. 4392-4440.

Nonner, W., D. Gillespie, and B. Eisenberg, How Do Long Pores Make Better K Channels? . Biophysical Journal, 2006. **90**: p. 239a.

Boda, D., W. Nonner, M. Valisko, D. Henderson, B. Eisenberg, and D. Gillespie, Steric Selectivity in Na Channels Arising from Protein Polarization and Mobile Side Chains*.* Biophys. J., 2007. **93**(6): p. 1960-1980.

Boda, D., M. Valisko, B. Eisenberg, W. Nonner, D. Henderson, and D. Gillespie, The combined effect of pore radius and protein dielectric coefficient on the selectivity of a calcium channel*.* Physical Review Letters, 2007. **98**: p. 168102.

Eisenberg, B. and W. Nonner, Shockley-Ramo theorem measures conformation changes of ion channels and proteins*.* Journal of Computaional Electronics, 2007. **6**: p. 363-365.

Boda, D., W. Nonner, D. Henderson, B. Eisenberg, and D. Gillespie, Volume Exclusion in Calcium Selective Channels*.* Biophys. J., 2008. **94**(9): p. 3486-3496.

Boda, D., W. Nonner, M. Valisko, D. Henderson, B. Eisenberg, and D. Gillespie, 2222-Pos Competition of Steric repulsion and Electrostatic Attraction in the Selectivity Filter of Model Calcium Channels*.* Biophys. J., 2008. **94**(1\_MeetingAbstracts): p. 2222-.

Roth, R., D. Gillespie, W. Nonner, and B. Eisenberg, Bubbles, Gating, and Anesthetics in Ion Channels*.* Biophys. J., 2008. **94** p. 4282-4298.

Boda, D., M. Valisko, D. Henderson, B. Eisenberg, D. Gillespie, and W. Nonner, Ionic selectivity in L-type calcium channels by electrostatics and hard-core repulsion*.* J. Gen. Physiol., 2009. **133**(5): p. 497-509.

Eisenberg, B., D. Boda, J. Giri, J. Fonseca, D. Gillespie, D. Henderson, and W. Nonner, Self-organized Models of Selectivity in Ca and Na Channels*.* Biophysical Journal, 2009. **96**(3): p. 253a.

Malasics, A., 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*.* Biochim Biophys Acta, 2009. **1788**: p. 2471-2480.

**Gillespie work on Density Functional Theory, ICC, etc.**

Gillespie, D., Toward making the mean spherical approximation of primitive model electrolytes analytic: An analytic approximation of the MSA screening parameter*.* J Chem Phys, 2011. **134**(4): p. 044103-3.

Malasics, A., D. Boda, M. Valisko, D. Henderson, and D. Gillespie, Simulations of calcium channel block by trivalent cations: Gd(3+) competes with permeant ions for the selectivity filter*.* Biochim Biophys Acta, 2010. **1798**(11): p. 2013-21.

Gillespie, D., Analytic Theory for Dilute Colloids in a Charged Slit*.* The Journal of Physical Chemistry B, 2010. **114**(12): p. 4302-4309.

Gillespie, D., J. Giri, and M. Fill, Reinterpreting the Anomalous Mole Fraction Effect. The ryanodine receptor case study. Biophyiscal Journal, 2009. **97**(8): p. pp. 2212 - 2221

Malasics, A., D. Gillespie, and D. Boda, Simulating prescribed particle densities in the grand canonical ensemble using iterative algorithms*.* Journal of Chemical Physics, 2008. **128**: p. 124102.

Gillespie, D. and M. Fill, Intracellular Calcium Release Channels Mediate Their Own Countercurrent: The Ryanodine Receptor Case Study*.* Biophys. J., 2008. **95**(8): p. 3706-3714.

Gillespie, D., 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*.* Biophys. J., 2008. **95**(2): p. 609-619.

Gillespie, D. and D. Boda, The Anomalous Mole Fraction Effect in Calcium Channels: A Measure of Preferential Selectivity*.* Biophys. J., 2008. **95**(6): p. 2658-2672.

Gillespie, D., Energetics of divalent selectivity in a calcium channel: the ryanodine receptor case study*.* Biophys J, 2008. **94**(4): p. 1169-84.

Valisko, M., D. Boda, and D. Gillespie, Selective Adsorption of Ions with Different Diameter and Valence at Highly Charged Interfaces*.* Journal of Physical Chemistry C, 2007. **111**: p. 15575-15585.

Xu, L., 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, 2006. **90**: p. 443-453.

Wang, Y., L. Xu, D. 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, 2005. **89**: p. 256-265.

Roth, R. and D. Gillespie, Physics of Size Selectivity*.* Physical Review Letters, 2005. **95**: p. 247801.

Gillespie, D., L. Xu, Y. Wang, and G. Meissner, (De)construcing the Ryanodine Receptor: modeling ion permeation and selectivity of the calcium release channel*.* Journal of Physical Chemistry, 2005. **109**: p. 15598-15610.

Gillespie, D., M. Valisko, and D. Boda, Density functional theory of the electrical double layer: the RFD functional*.* Journal of Physics: Condensed Matter 2005. **17**: p. 6609-6626.