Crowded Charges Bibliography

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Early Papers

Predecessor Papers in the context of PNP (not crowded charges, not L type Ca^{2+} 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 Ca^{2+} 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.

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

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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.

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