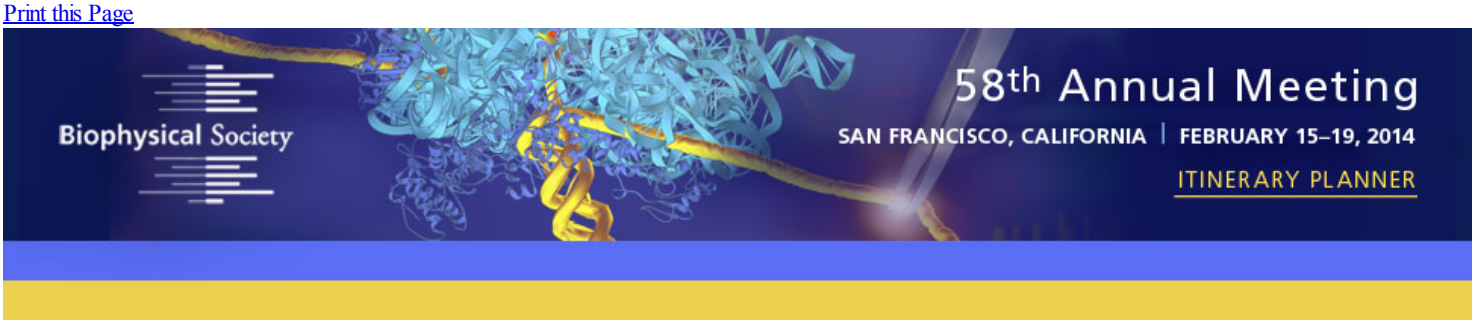
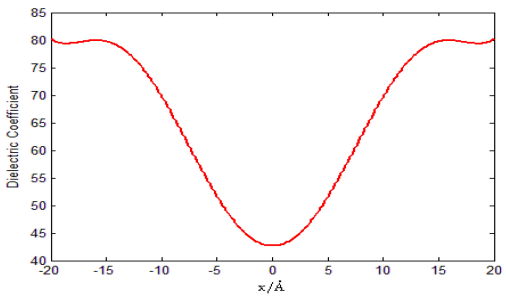


Biophysical Journal 106(2) pp. 133a - 134a

Presentation Abstract

Session Title:	Voltage-gated Ca Channels I
Location:	Hall D
Presentation Number:	686-Pos
Board Number:	B441
Presentation Time:	2/16/2014 1:45:00 PM
Abstract Title:	POISSON-FERMI MODEL OF A CALCIUM CHANNEL: CORRELATIONS AND DIELECTRIC COEFFICIENT ARE COMPUTED OUTPUTS.
Author Block:	**Bob Eisenberg**[1], Jinn-Liang Liu[2]. [1]Rush University, Chicago, IL, USA, [2]National Hsinchu University of Education, Hsinchu, Taiwan.
Abstract Body:	We derive a continuum model of biological calcium channels, called the **Poisson-Fermi equation**, designed to deal with crowded systems in which ionic species and side chains nearly fill space. The model is evaluated in three dimensions. It includes steric and correlation effects and is derived from classical hard-sphere lattice models of the configurational entropy of spherical ions and solvent molecules. Formulae are given for all ionic species with different sizes and valences. Unphysical overcrowding does not occur with Fermi distributions, unlike with Boltzmann distributions. We provide an analytical description of the implicit dielectric ('primitive') model of electrolytes that yields global and local formulae for chemical potential. Poisson-Fermi equations are local, with different correlations at different places. Correlations produce spatial variations of dielectric permittivity as an output of analysis. Computations of binding are consistent with Monte Carlo binding curves. They have anomalous mole fraction effects, an effective blockage of sodium binding by a tiny concentration of calcium ions. Symbols and details in J.Computational Physics **2013**, *15*, 88; J Phys Chem B **2013** doi:10.1021/jp408330f

$$\varepsilon_w(l_c^2\nabla^2-1)\nabla^2\varphi=\sum_{i=1}^{K}q_iC_i=\rho. \quad \textbf{OR} \quad \varepsilon_w(l_c^2\nabla^2-1)\Psi=\rho;\ \nabla^2\varphi=\Psi.$$



Commercial Relationship:	**B. Eisenberg:** None. **J. Liu:** None.

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