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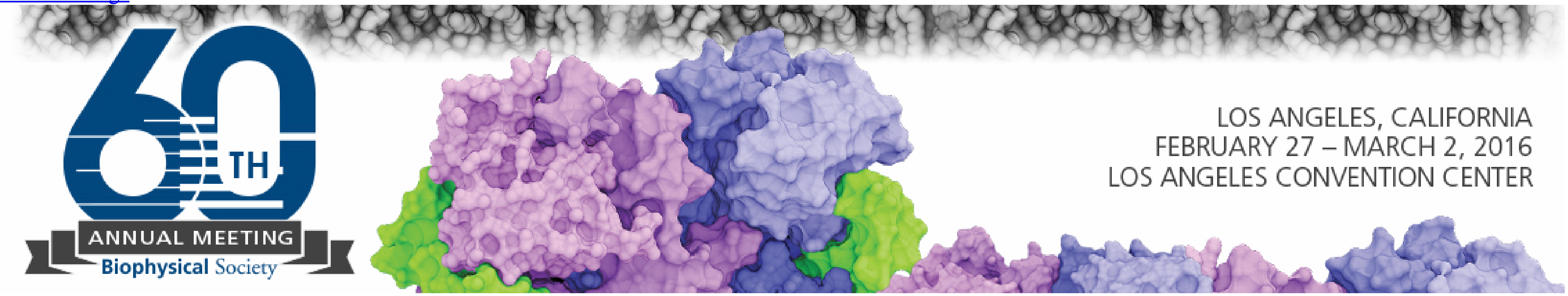

Presentation Abstract

Session Title:	Voltage-gated K Channels and Mechanisms of Voltage Sensing and Gating (Late)
Location:	West Hall
Presentation Number:	L3306-Pos
Board Number:	LB66
Presentation Time:	2/28/2016 1:45:00 PM
Abstract Title:	ON THE CONDUCTIVITY AND SELECTIVITY PARADOX IN BIOLOGICAL CHANNELS
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Abstract Body:	We address the paradox [1] of alike charge selectivity and conductivity of ion channels: why the high affinity at the biding site required for selectivity does not retard conduction through the pore. We use a model of a selectivity filter with four binding sites to propose a resolution of the paradox, based on physical first principles. We derive equilibrium distributions of potassium and sodium ions in a negatively-charged filter coupled to a bath. Each type of ion has a specific chemical potential both in the channel and in the bath. We analyze the energy levels in this system and show that, for a given set of parameters, the most probable states involve at least two K ions and allow maximum 3 ions to be present in the filter. We derive a reduced grand-canonical ensemble for a variable number of ions in the filter with two K ions in it as the ground state. We use linear response theory to estimate analytically K and Na currents through the channel in the single-file approximation of the knock-on mechanism of conduction. We show that the combination of dehydration and the self-induced electrostatic energy barrier (due to ionic Coulomb blockade [2]) results naturally in strong selectivity and high conductivity of strongly-charged narrow filter. We introduce a set of master equations for simultaneous transition through the channel of the

two types of alike ions and provide a numerical example demonstrating strong selectivity between ions and a conductivity approaching diffusion limit. In conclusion, we discuss the mechanisms of dehydration and the role of the filter wall fluctuation within the proposed theoretical model of optimal conduction and selectivity.

[1] MacKinnon, R. (2003). FEBS Letters, 555(1), 62-65.
[2] Kaufman, I. et al. (2013). Physical Review E, 88(5), 52712.

Commercial Relationship: **D.G. Luchinsky:** None. **W... Gibby:** None. **I.K. Kaufman:** None. **R.S. Eisenberg:** None. **P.V. McClintock:** None.