Presentation Abstract

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Abstract Title: ON THE CONDUCTIVITY AND SELECTIVITY PARADOX IN BIOLOGICAL CHANNELS

Author Block: Dmitry G. Luchinsky¹, Will A.T. Gibby¹, Igor Kh Kaufman¹, Robert S. Eisenberg², Peter V.E. McClintock¹.
¹Physics, Lancaster University, Lancaster, United Kingdom, ²Molecular Biophysics & Physiology, Rush University, Chicago, IL, USA.

Abstract Body: We address the paradox [1] of alike charge selectivity and conductivity of ion channels: why the high affinity at the binding 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.
