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COMPOSE

Out of the blue.....by way of John Prausnitz.....Re: Schroedinger Equation

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Bob Eisenberg -beisenbe@rush.edu- to alder1, John, bcc: Chun, bcc: Rich, bcc: Ardyth

6:11 AM (7 minutes ago)

Dear Dr. Alder, or Beml, if first names are OK,

John Prausnitz kindly suggested that I should contact you about some ideas and work of mine and some separate work of a fine mathematician Chun Liu.

To avoid confusion in this email I will only talk of my work on enzyme catalytic sites and of some ideas it provoked in me.

For years I have worked on ion channels (see attached CV also as a professional introduction) and have eventually had some success in understanding the selectivity of calcium channels (e.g., of the heart) and sodium channels (of nerve).

The key to understanding the selectivity of these channels is the high density of fixed charge in the walls of their very tiny pores. ('channels' in this world refers to the protein and not the pore down the middle of the channel protein). This charge arises in the acid side chains of the amino acids (glutamate and aspartate) and for the sodium channel also the basic side chain lysine. For us biophysicists, acid = negative fixed charge (crudely speaking) basic = positive fixed charge

The number density in chemical units is some 20 molar (no that is not a misprint). For reference solid NaCl is 37 molar.

Densities of this order are actually observed in crystal structures of other types of channels.

Motivated by this work, Jie Liang, his student David Jimenez-Morales, and I decided to examine ENZYMES of known crystal structure to see what the density of fixed charge is in their active sites, where