Bob Eisenberg <bob.eisenberg@gmail.com>

Moving forward....

Bob Eisenberg <bob.eisenberg@gmail.com> Tue, May 27, 2014 at 7:28 AM
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Dear Zuzanna

I just read your article in PCCP about conical nanopores and the exciting news about your MsSimPore package.

I am writing hoping that I can persuade you to move forward so the package can allow treatment of solutions as they really are, with nonideal properties.

I attach a few articles I have written on this subject but suspect you do not need to read them. They do provide abundant documentation of experiments that support my list of statements below.

You know quite well I suspect that

a) only monovalent monovalent solutions below some 20 mM follow Poisson Boltzmann or Debye Huckel even approximately. These of course are NOT ideal since their free energy goes as the sq root and not linearly with concentration

b) No divalent solutions are even approximately described by PB or DH.

c) No mixtures are even approximately described by PB or DH

d) ALL of life (no exceptions known) occurs in ionic mixtures in which calcium plays an important, usually vital role

e) technology (e.g., at working electrodes) and life (in and near active sites, ion channels, nucleic acids) involve concentrations much more than 1 molar, and are nothing at all like ideal

f) the excess free energy in all these cases is large often more than 50% of the total free energy (per mole).

g) the excess free energy in all these cases is a function of ALL concentrations, and often a sensitive function. So the driving force (i.e., gradient of electrochemical potential) for sodium would depend on ALL ions. Thus SODIUM current through a PERFECTLY SELECTIVE channel would depend on the concentrations of all ions, not just sodium.

h) there are several versions of the all spheres model of ionic solutions that deal with these nonideal interactions, one of which Martin Burger has coded very well indeed.

It seems to me crucial that the field of nanochannels not go the path of nonsense and assume that all solutions follow Poisson Boltzmann or worse are ideal.

Do you agree?

If so, what can we do to prevent everyone doing the easy thing, which is of course natural, but simply does not describe how almost all ionic solutions behave, whether in bulk or in channels, of any size.

As ever
Bob

PS I attach a few papers on these subjects, including
a direct experimental measurement of the ionizable sites
at active sites of enzymes. Also a CV so you can see what
we have been up to lately.

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12 attachments

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