Poster-Board Number **B270**
Presentation Number **1293-Pos**

Presentation
Feb 29, 2016
Monday 1:45 pm

Poisson-Fermi Model of the Ion-exchange Mechanism of the SODIUM/CALCIUM exchanger NCX

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Abstract

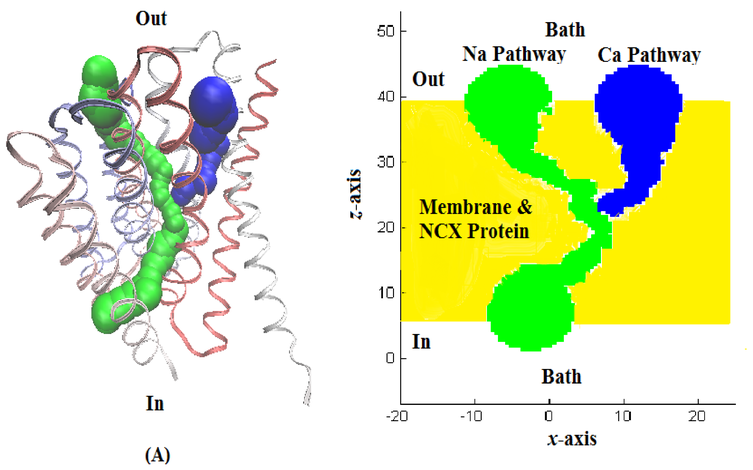
Ion-exchange mechanism of **the NCX transporter** crystallized by **Liao**, *Li, Zeng, Sauer, Belmares, and Jiang* ***Science (2012)*** *335:686* is studied using the **Fermi Poisson theory** developed by **Jinn Liang Liu**, Journal of Computational Physics (2013) 247:88 and **Jinn Liang Liu and Bob Eisenberg**

Journal of Physical Chemistry B (2013) 117:12051
J Chem Phys (2014) 141:07510; J Chem Phys (2014) 141:22D532 arXiv:1506.06203
Physical Review E (2015) 92: 012711 arXiv: 1506.05953
Chemical Physics Letters (2015) 637:1

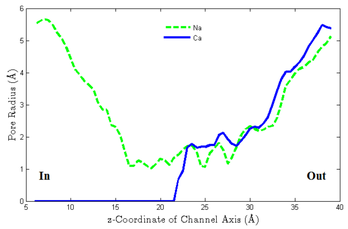
The theory considers the **steric effect of ions and water** molecules with different sizes and **interstitial voids**, the correlation effect of crowded ions with different valences, and the screening effect of **polarized water molecules** in an inhomogeneous aqueous electrolyte.

We calculate the electrostatic and steric potentials of the **four binding sites in NCX**, i.e., three Na^+ binding sites and one Ca^{2+} binding site, with protein charges provided by the software ***PDB2PQR***. The energy profiles of Na^+ and Ca^{2+} ions along their respective Na^+ and Ca^{2+} pathways in experimental conditions enable us to explain the fundamental mechanism of NCX that extrudes intracellular Ca^{2+} across the cell membrane against its chemical gradient by using the downhill gradient of Na^+. Atomic and numerical details of the binding sites are given to illustrate the ion-exchange mechanism.

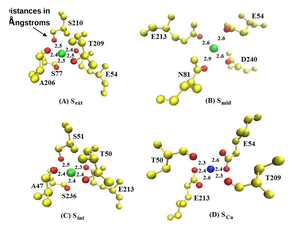
Structure



Winding Tortuous Irregular Pore

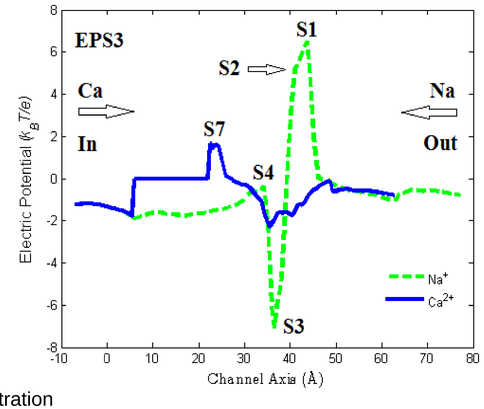


Binding Sites

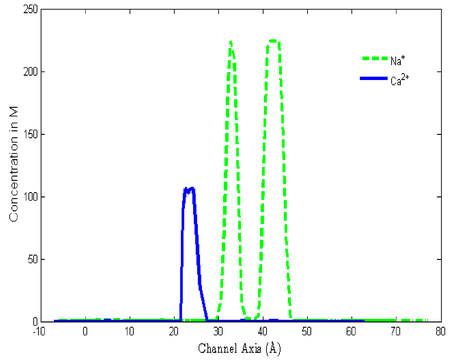


Electrical Potential and Concentration Profiles

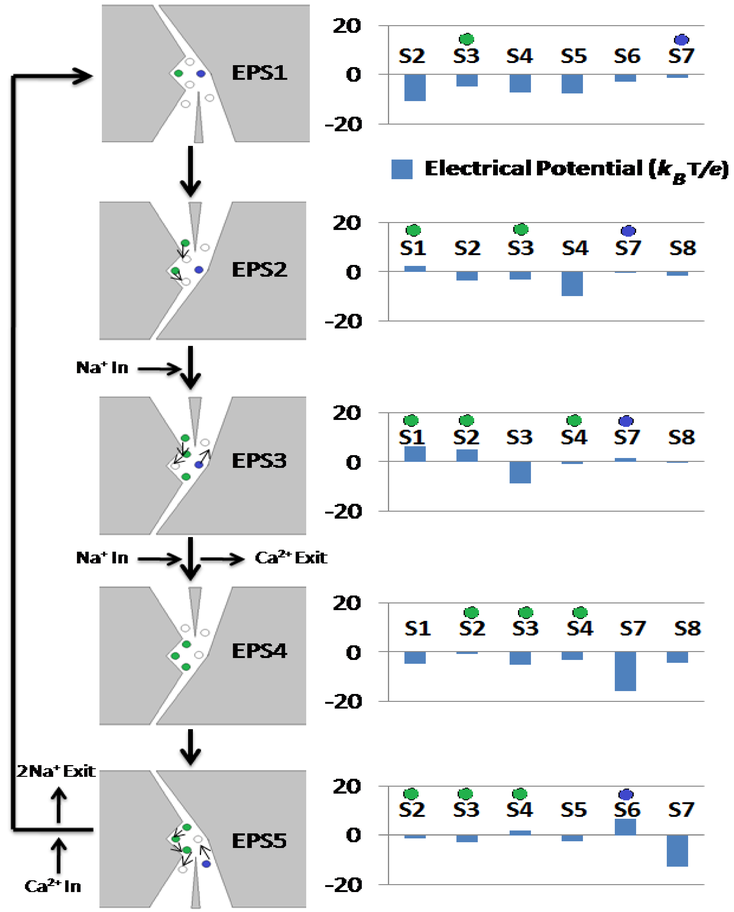
Electrical Potential



Concentration



Energies of Binding Sites computed as outputs of Fermi Poisson



Fermi (like) Distribution

$$C_i(\mathbf{r}) = C_i^{bath} \exp\left(-\beta_i \phi(\mathbf{r}) + S^{steric}(\mathbf{r})\right)$$

$S^{steric}(\mathbf{r}) = \ln(\Gamma(\mathbf{r}) / \Gamma(bath))$
$\Gamma(bath)$ = volume fraction of voids in bath
$\Gamma(\mathbf{r})$ = volume fraction of voids in channel

Explicit formulae in publications
e.g., Phys Rev E (2015) 92: 012711