Poster Board DB2b
Session 450:
Computation Tools

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

Presentation Number:
450.09
Mon Oct 19: 1-2 pm

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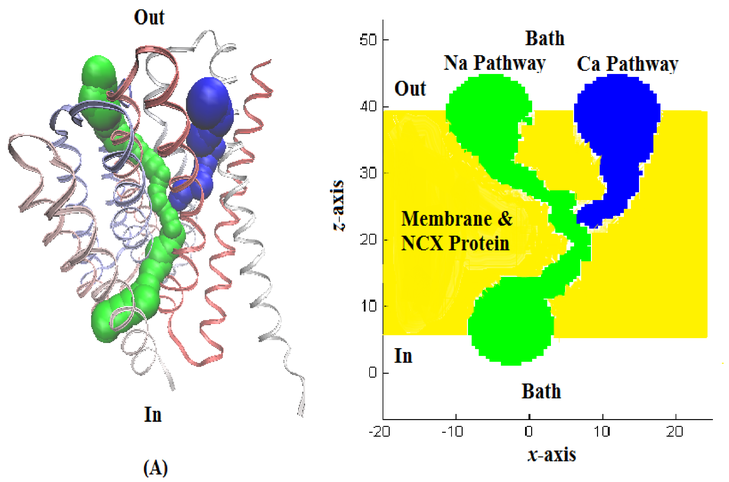
Abstract

The 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 (2013) B 117:12051
J ChemPhys (2014) 141:07510 J ChemPhys (2014) 141:22D532 arXiv:1506.06203
Physical Review E (2015) 92: 012711 arXiv: 1506.05953
Chemical Physics Letters (2015) 637:1

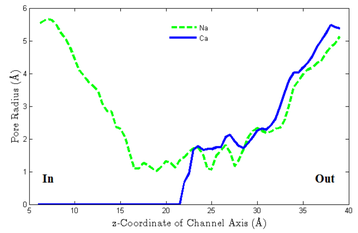
The theory considers the steric effect of ions and water molecules with different sizes and interstitial voids, the correlation effect of crowded ions with different valences, and the screening effect of polarized water molecules in an inhomogeneous aqueous electrolyte.

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.

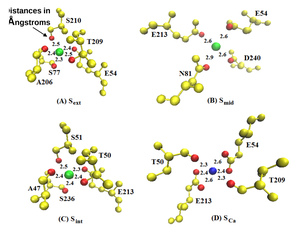
Structure



Winding Tortuous Irregular Pore

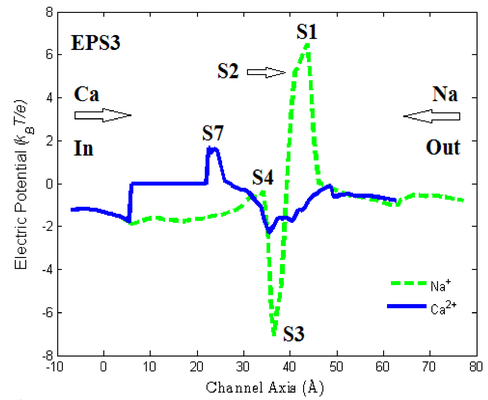


Binding Sites

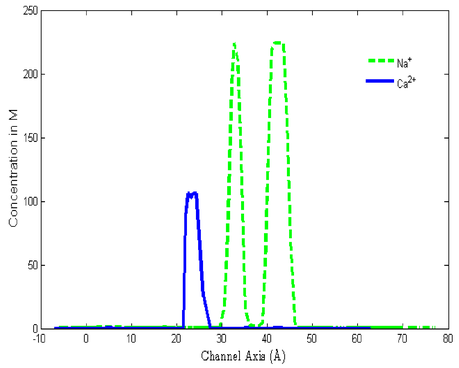


Electrical Potential and Concentration Profiles

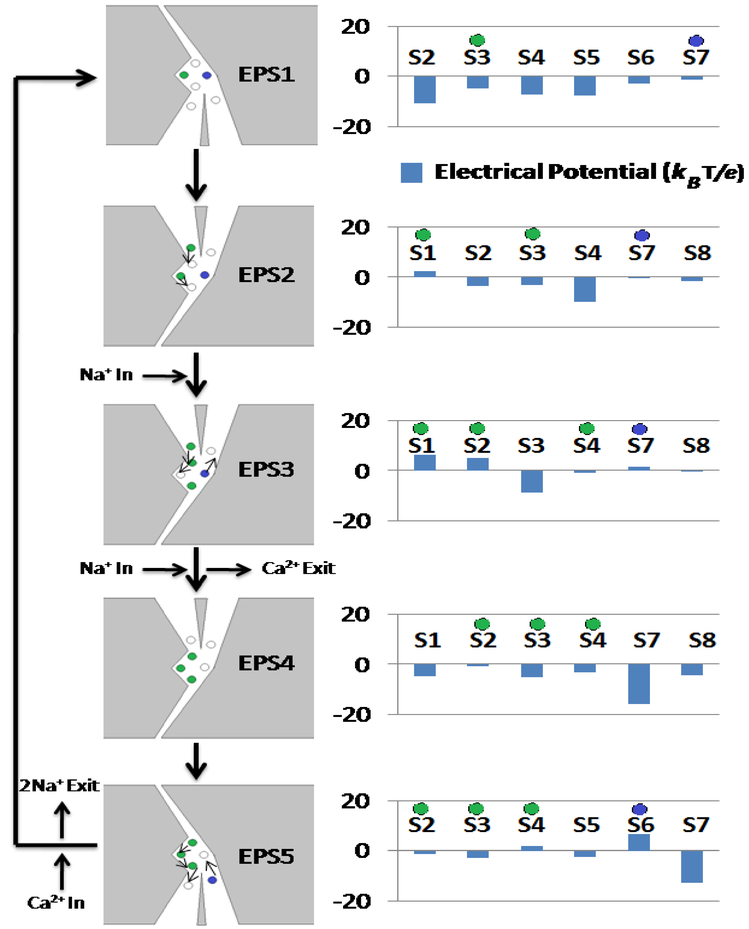
Electrical Potential



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