Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Strontium and Barium in aqueous solution and an ion channel blocking site. MANGESH CHAUDHARI, SUSAN REMPE, Sandia National Labs — Ion hydration structure and free energy establish criteria for understanding selective ion binding in potassium (K+) ion channels, and may be significant to understanding blocking mechanisms as well. Recently, we investigated the hydration properties of Ba2+, the most potent blocker of K+ channels among the simple metal ions. Here, we use a similar method of combining ab-initio molecular dynamics simulations, statistical mechanical theory, and electronic structure calculations to probe the fundamental hydration properties of Sr2+, which does not block bacterial K+ channels. The radial distribution of water around Sr2+ suggests a stable 8-fold geometry in the local hydration environment, similar to Ba2+. While the predicted hydration free energy of -331.8 kcal/mol is comparable with the experimental results of -334 kcal/mol, the value is significantly more favorable than the -305 kcal/mol hydration free energy of Ba2+. When placed in an innermost K+ channel blocking site, the solvation free energies and lowest energy structures for both Sr2+ and Ba2+ are nearly unchanged compared with their respective hydration properties. That result suggests that difference in blocking behavior may arise due to kinetic properties associated with exchange of water ligands for channel ligands instead of equilibrium thermodynamic properties.

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Date submitted: 06 Nov 2015 Electronic form version 1.4