192a MD Simulations of Water and Sodium Counter-Ion Diffusion in the Pores of Beta - Lactoglobulin Crystals

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We carried out 5 ns molecular dynamics (MD) simulations of water and sodium counter-ions (Na^+) in a C2221 orthorhombic β-lactoglobulin crystal. The pores have a diameter of 1.26–2.10 nm. Water molecules close to the protein surface are found to diffuse in an anomalous way, while the diffusion of water in the core of the zig-zag pores is classical. The diffusivity of water molecules in the core zone is about 1/6th of the diffusivity of free water. There is qualitative agreement with QENS experiments.

The fluctuations of the protein atoms have a significant effect on the value of the water diffusivity, which increases from about 0.65 to 0.89 nm^2/ns when fluctuations are accounted for. Lysine residues in the constricted zones of the pores (positively charged lys70) are the main obstacles to water and ion diffusion. Therefore, simulations with position restraints on the protein atoms do not provide a correct picture of the diffusion behavior. Removing the position restraints on the lysine residues also leads to a significant increase in the sodium ion mobility. The motion of the ions appears anomalous on the timescale of the simulations; the long-time behavior of the counterion diffusion is not clear yet.

The results are not only of interest to study ion and water transport through biological nanopores, but may also elucidate water-protein and ion-protein interactions in protein crystals.