

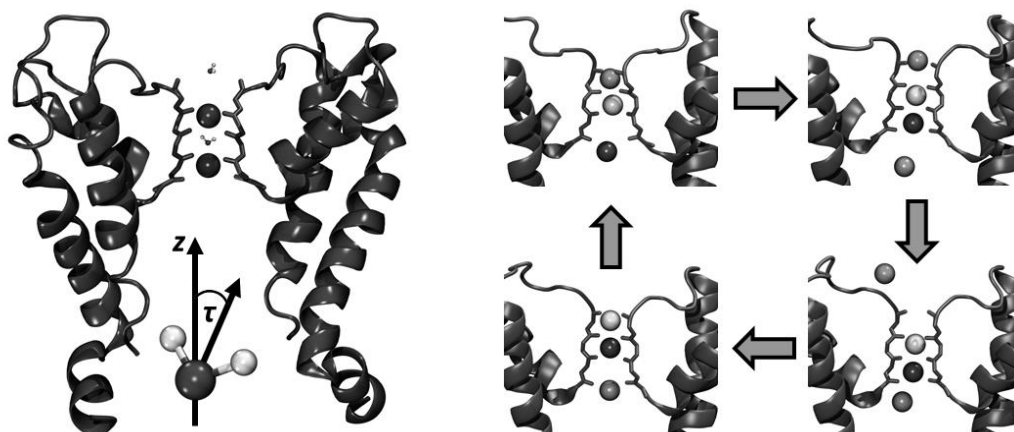
Analysis of gating behavior and microscopic water structure in small viral K⁺-ion channels

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Ion channels fluctuate stochastically between “open” and “closed” states, which determine the ion flux through biological membranes, also known as “gating”. This crucial feature of ion channels is necessary in cellular, biological systems to regulate the ion concentration level, which is essential for the processes of homeostasis or second messaging. Yet the origin of gating is not fully understood. The structure of a channel in its various gating states, which is controlled by its amino acid sequence, also plays a vital role for ion selectivity. We here focus on tetrameric potassium channels, for which very short, miniature systems exist. These ideal model systems, KCV_{PBCV-1} and KCV_{ATCV-1} that are found in *chlorella* viruses are comprised of only 94 and 82 amino acids per monomer [1-4] and play an important role for determining elementary structure-function relations. Although these channels are comparably small, they show all essential features like gating and selectivity.



A commonly used method for investigation of ion channels in a membrane domain is molecular dynamics (MD) simulation. Modern computer hardware allows for simulations up to microsecond timescales, in which multiple ion transitions are observable. To quantify the transition process relevant descriptors need to be developed. Ion transitions could correlate with structured ion and water distributions inside the channel cavity, dominated by confinement effects and water-ion interactions. To gain insight into these interactions we present a computational approach based on WaterDynamics [5] to determine the orientation of water molecules with respect to the channel axis for different trajectories showing various conduction characteristics. To analyze the orientation of intra-cavity solvent molecules the local solvent densities are calculated and combined with the probability density of water orientations and positions. The approach is applied to long MD trajectories and analyzed for different phases of the transitions composed of resting and rapid conductance states.

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