

## Distinguished Lecture Series in Physiology

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## “Studying ion channels using two-dimensional vibrational spectroscopy”

Growing Potassium ( $K^+$ ) ion channels are transmembrane proteins that regulate the passage of  $K^+$  ions through cell membranes. The selectivity filter is the narrowest part of the pathway of ions through the channel. It plays a determining role in the remarkably high ion selectivity and transport rates. Despite decades of work the precise mechanistic details of the transport through ion channels are still elusive. According to the so-called soft-knock mechanism water molecules alternate between  $K^+$  ions in the selectivity filter and co-transport with the ions. In contrast, the hard-knock mechanism assumes that water is absent from the selectivity filter during ion conduction. Two-dimensional infrared spectroscopy (2D IR) is an ultrafast technique that measures molecular vibrations. Carbonyl stretching vibrations of a protein backbone are sensitive probes of the local chemical environment and can be used to discriminate between water and  $K^+$  ions in the selectivity filter. I will present our recent line shape simulations and experiments, performed by our collaborators, on a prokaryotic  $K^+$  channel KcsA. Our results are clearly consistent with all the previous 2D IR experiments and illustrate the prevalence of the soft-knock ion configurations in the closed conductive state of the KcsA channel. Additionally, I will discuss our most recent simulations and 2D IR experiments reporting on ion and water dynamics as well as the difference in binding between  $K^+$  and competing  $Na^+$  ions.

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GBSF and Zoom  
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