Abstract Submitted
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Connecting ion channel simulations to experiment PETER HUGO NELSON, Benedictine University — A simple theoretical framework is used to connect MD simulation with ion channel permeation experiments. MD simulations of potassium channels typically exhibit at least two stable selectivity filter states, one with double occupancy and another with triple occupancy. In the association/dissociation (A/D) model, transitions between these two states occur via concerted motion of all three ions in a shunt-on shunt-off mechanism that is consistent with a large group of published MD simulations. This is the simplest model that explains the universal saturating behavior observed experimentally for many ion channels. Published permeation experiments through the MaxiK channel over a wide range of concentrations and positive voltages are shown to be remarkably consistent with the predictions of this model. Published MD simulations of the Kv1.2 potassium channel exhibit an extended shunt-on shunt-off mechanism at one end of the selectivity filter and a pop-off pop-on mechanism at the other end. This two-step mechanism is incorporated into an asymmetric variant of the A/D model that successfully explains published permeation data through the Shaker potassium channel at physiological concentrations, and successfully predicts qualitative changes in the negative current-voltage data (including a transition to super-Ohmic behavior) based solely on a fit to positive voltage data (that appear linear). Support from NSF 0836833 is gratefully acknowledged.

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