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Zilong Song*, zilong.song@ucr.edu, and **Xiulei Cao, Tzyy-Leng Horng and Huaxiong Huang**. *Selectivity of the KcsA potassium channel: Analysis and computation.*

Ion channels regulate the flux of ions through cell membranes and play significant roles in many physiological functions. In this talk, we present an analytical and computational study of a mathematical model of the KcsA potassium channel, including the effects of ion size (Bikerman model) and solvation energy (Born model). Under equilibrium conditions, we obtain an analytical solution of our modified PNP system, which is used to explain selectivity of KcsA of various ions (K^+ , Na^+ , Cl^- , Ca^{2+} and Ba^{2+}) due to negative permanent charges inside the filter region and the effect of ion sizes. Our results show that K^+ is always selected over Na^+ , as smaller Na^+ ions have larger solvation energy. As the amount of negative charges in the filter exceeds a critical value, divalent ions (Ca^{2+} and Ba^{2+}) can enter the filter region and block the KcsA channel. For the non-equilibrium cases, due to difficulties associated with a pure analytical or numerical approach, we use a hybrid analytical-numerical method to solve the modified PNP system. Our predictions of selectivity of KcsA channels and saturation phenomenon of the current-voltage (I-V) curve agree with experimental observations. (Received September 14, 2019)