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Snug-fit, fluctuations, and metal-ion hydration in the selectivity of potassium ion channels

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On the basis of molecular simulation, an identification of a single dominating physical factor responsible for Na+/K+ selectivity of the KcsA channel has been contentious. The potential distribution theorem and quasi-chemical theory cast new light on the factors responsible for Na+/K+ selectivity. In that context, we argue that an alternative definite formulation of the molecular statistical thermodynamic problem can help in achieving a concensus view of selectivity. We summarize the necessary new theoretical ingredients and published numerical results in working toward that concensus view.