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Ion Discrimination by Nanoscale Design[1] SUSAN REMPE, DAVID ROGERS, Sandia National Labs — Proteins that form membrane-spanning channels excel at discriminating between molecules on the basis of subtle structural and chemical differences. For example, some channels distinguish between water and ions; others between Na+ (sodium) and K+ (potassium) despite identical charges and only sub-Angstrom differences in size. If we could understand these structure/function relationships, we could potentially harness biological design principles in robust nanoscale devices that mimic biological function for efficient separations. Using ab initio molecular simulations, we have interrogated the link between channel structure and selective transport, both in cellular channels and polymer membranes. Our results emphasize the surprisingly important role of the environment that surrounds ion-binding sites, as well as the coordination chemistry of the binding site for raising or lowering the free energy barrier to transport in both systems.

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