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The Dependence of Ionic Conduction on the Dielectric Properties of Ion Channels MARCO SARANITI, DAVID MARREIRO, Illinois Institute of Technology, SHELA ABOUD, Worcester Polytechnic Institute — The ion channel OmpF porin is a water filled trimer found in the outer membrane of *Escherichia coli*. Each monomer is a hollow barrel structure with a physical constriction near the center that reduces the width of the pore to approximately 6 Å. Highly charged residues line the inside of the pore constriction, generating an intense electric field that facilitates the dynamics of ions through the channel. The cost of simulating these systems for long times is an oversimplification of key physical features of the ion channel system, most notably, the polarization effects related to the solvent (water) and the protein are poorly represented by a stepwise constant dielectric constant. While the use of this model for the aqueous solution inside the permeation pore is arguably suitable because the ionic hydration shell remains intact (at least away from the central constriction), its validity is questionable when used to describe the polarization response of the protein. In this work, a previously validated P^3M force-field scheme, self-consistently coupled to a Brownian Dynamics kernel, is used to investigate the influence of the protein dielectric constant on permeation in OmpF porin. The computed channel conductivity is in agreement with experimental measurements. Increased cation selectivity at low ionic concentrations is also observed in the simulations and appears to be dependent on the rings of aspartic acid residues around the mouths of the porin.

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