

Abstract Submitted
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Insight into the mechanics of the selectivity filter of *Escherichia coli* aquaporin Z¹ GUODONG HU, L.Y. CHEN, University of Texas at San Antonio — Aquaporin Z (AQPZ) is a tetrameric protein that forms water channels in *Escherichia coli*'s cell membrane. The histidine residue in the selectivity filter (SF) region plays an important role in the transport of water across the membrane. In this work, we perform equilibrium molecular dynamics (MD) simulation to illustrate influences of two different protonation states and the gate mechanics of the SF. We calculate the pore radii in the SF region versus the simulation time. We perform steered MD to compute the free energy profile, i.e., the potential of the mean force (PMF) a water molecule through the SF region. We calculate the binding energy of one water molecule with the SF region residues, using Gaussian. The hydrogen bonds formed between the side chains of Hsd 174 and side chains of Arg189 play important roles in the selectivity filter mechanics of AQPZ. The radii of the pores, hydrogen bond analysis, and free energies show that Hsd is favored than Hse.

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