Supporting Information for: Nanoscale Ion Pump Derived from a Biological Water Channel

Karl Decker,[†] Martin Page,[‡] and Aleksei Aksimentiev[*,†,¶]

Department of Physics, Engineer Research and Development Center, Construction Engineering Research Laboratory, US Army Corps of Engineers, and Beckman Institute for Advanced Science and Technology,

University of Illinois at Urbana–Champaign, Urbana, IL

E-mail: aksiment@illinois.edu, Telephone:+1-217-721-4764

[*]To whom correspondence should be addressed
[†]Department of Physics
[‡]Engineer Research and Development Center
[¶]Beckman Institute for Advanced Science and Technology

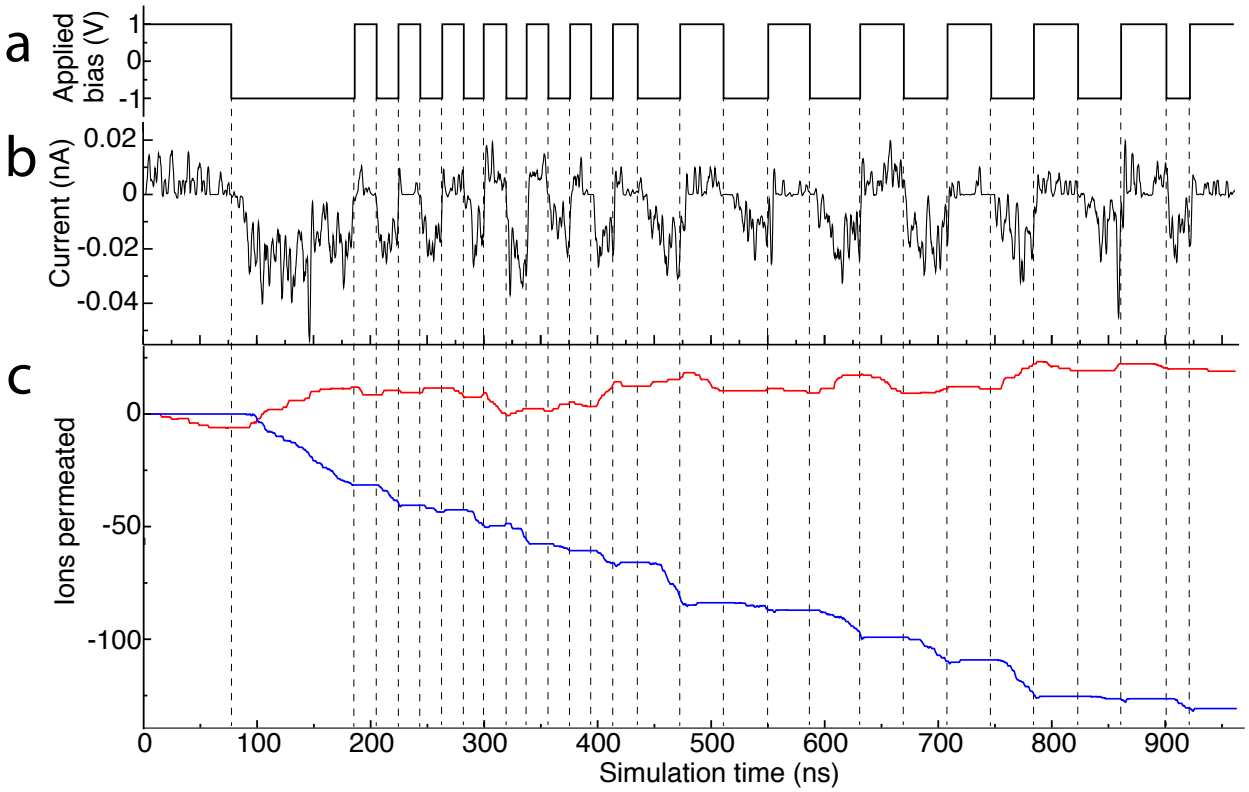


Figure S1: Current and ion permeation through truncated AQP at 1 V magnitude of applied bias. (a) Applied bias *versus* simulation time. Dashed lines serve as guides to the eye. (b) Ionic current through truncated AQP tetramer *versus* simulation time. The ionic current traces show 2 ns running average of the instantaneous current sampled every 9.6 ps. Dashed lines serve as guides for the eye. Positive current travels from *cis* to *trans* as defined main text Figures 1c. (c) The number of ions permeated across the truncated AQP tetramer system. Red traces indicate Cl^- permeation, blue traces indicate Na^+ permeation.

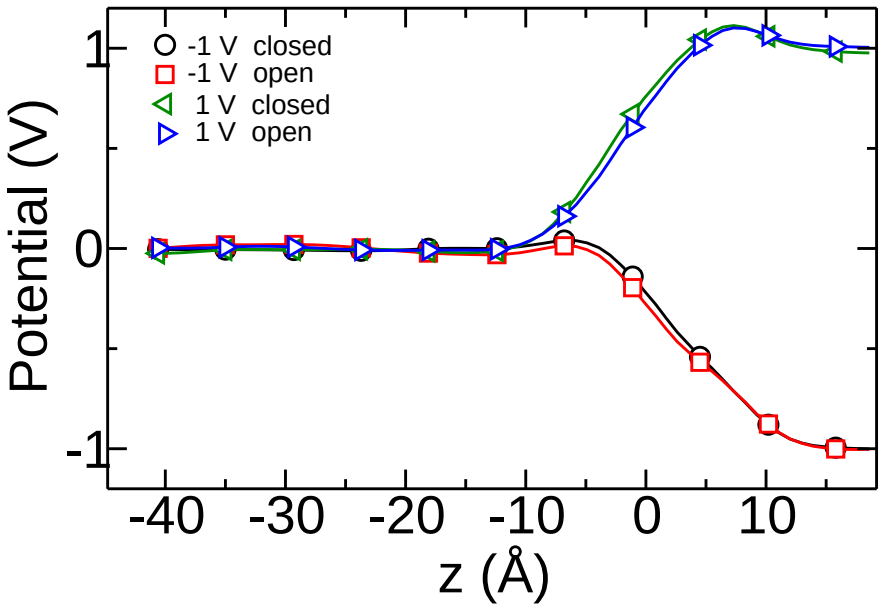


Figure S2: Profiles of electrostatic potential through truncated AQP pump in closed and open states. The electrostatic potentials were determined by first averaging the 3D maps of instantaneous electrostatic potentials over the frames of the MD trajectories that had one of the four channel monomers in either open or closed state (as defined by the z coordinate of the gate's guanadine group). The 1D profiles were extracted from the average 3D map along the z axis that passed through the crystallographic location of the center of mass of the channel's selectivity filter.

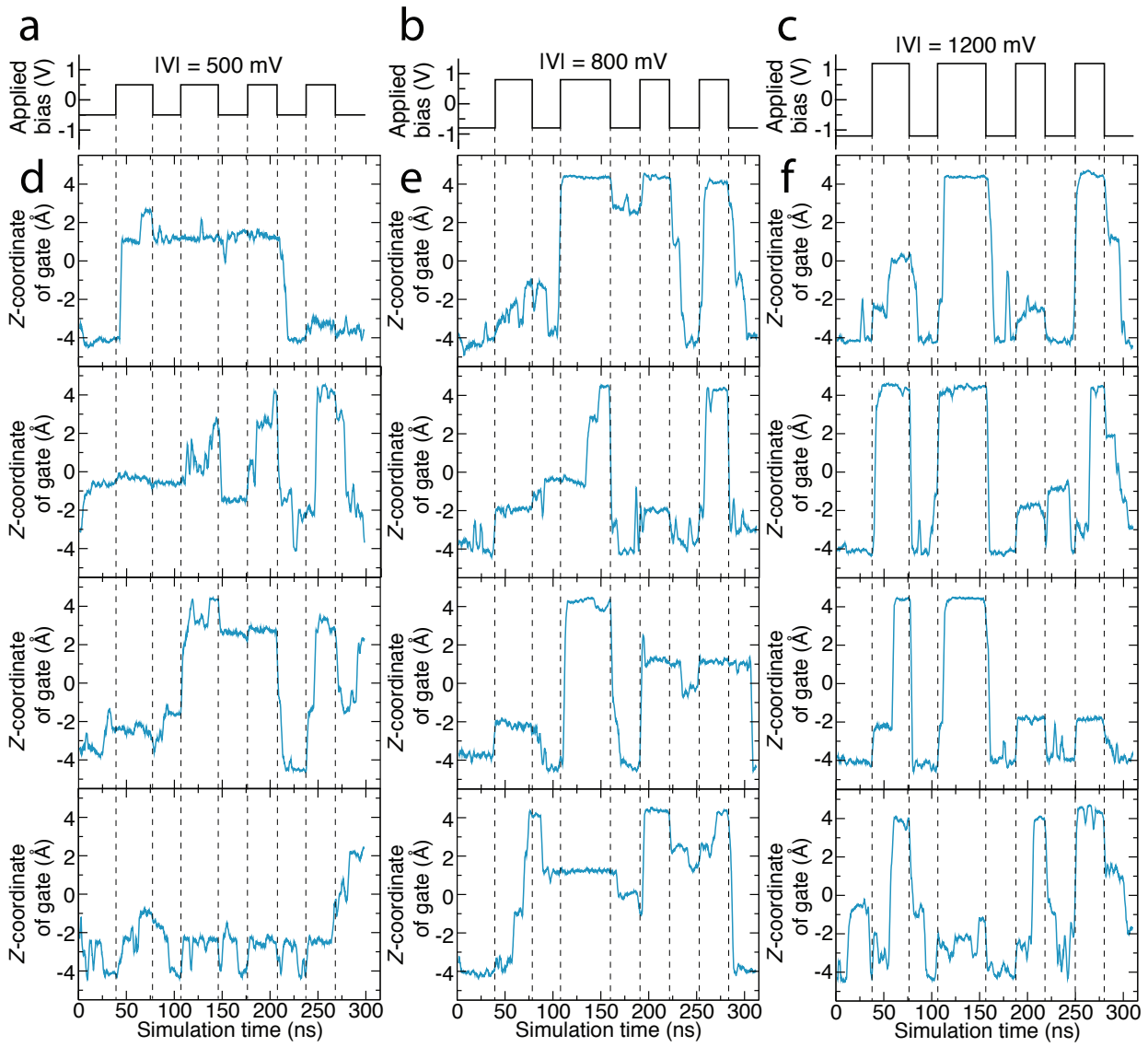


Figure S3: Behavior of the Arg-197 gate at 500 mV, 800 mV, and 1200 mV. The step functions in a-c show the applied transmenbrane bias over simulation time, while d-f show the response of the four gates in each tetramer at each magnitude of bias, as measured by the z-coordinate of the guanadine group of Arg-197. The guanadine group and the gate are represented in Figure 4e-f and Figure S5e-f.

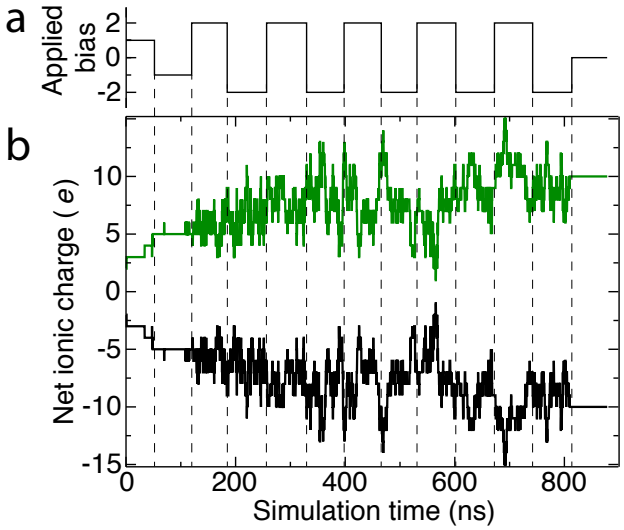


Figure S4: Ionic charge in the double-membrane truncated AQP system under ion pumping conditions. (a) Applied bias *versus* simulation time. Dashed lines serve as guides to the eye. (b) Net charge of ions in the anode (green trace) and cathode (black trace) chambers.

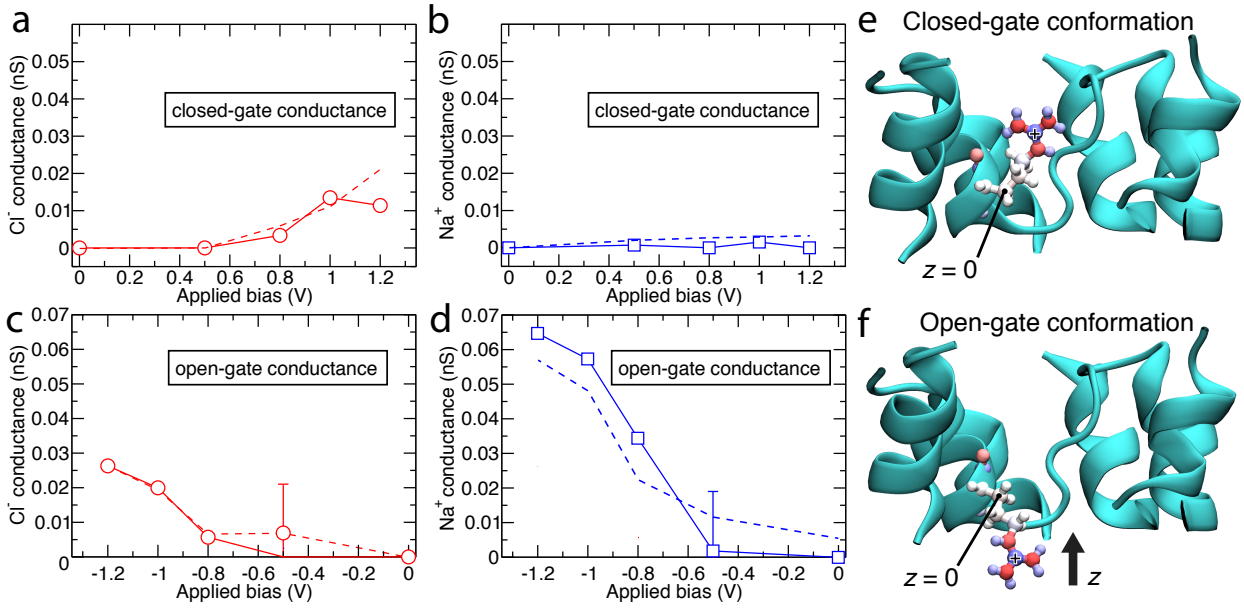
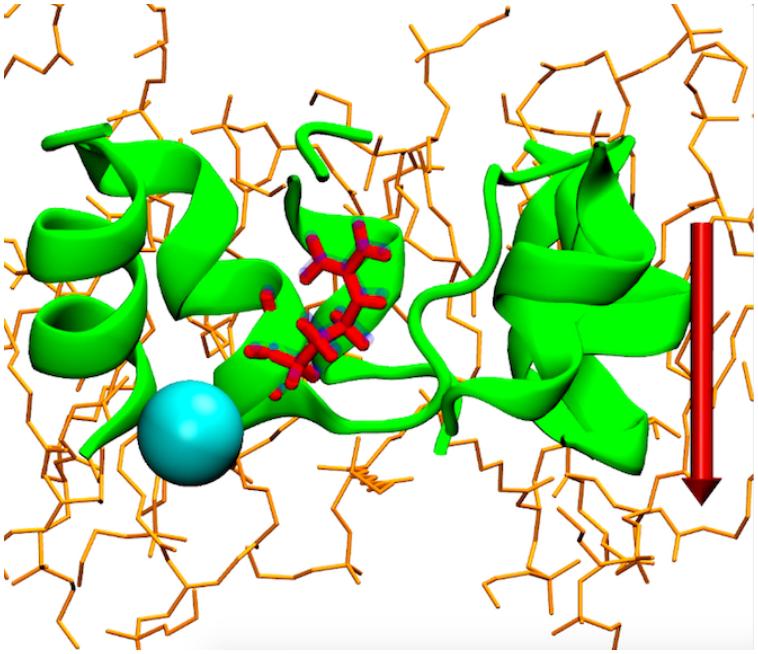
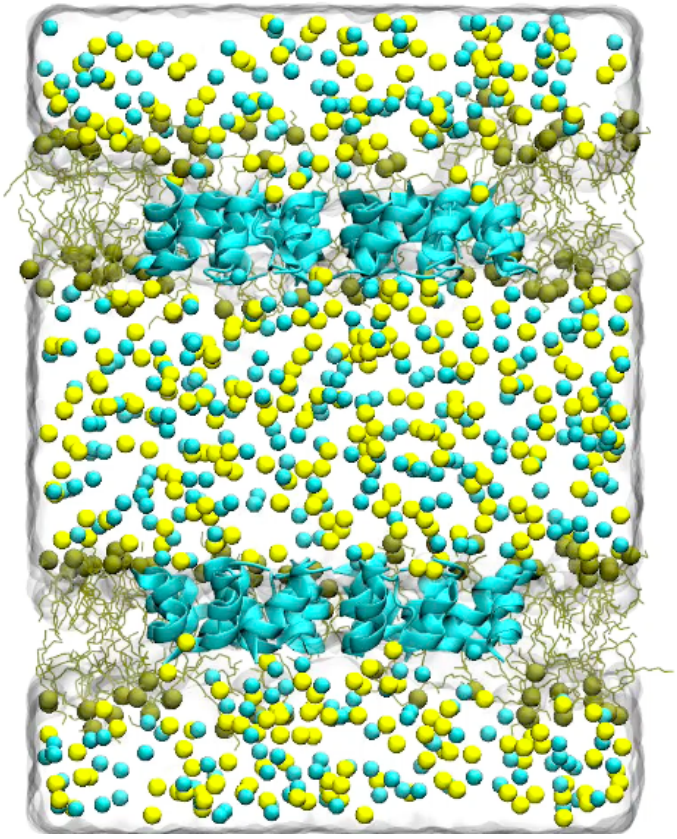


Figure S5: Mean current through truncated AQP monomers while the Arg-197 gate is closed (a-b, solid lines) and when it is fully open (c-d, solid lines); sample closed-gate (e) and open-gate (f) conformations are shown for context, as well as mean current per monomer regardless of the gate conformation (a-d, dashed lines). The Arg-197 gate was considered to be closed when the z-coordinate of its guanadine group, the terminal carbon of which is marked in (e) with a "+", was greater than 3.7 Angstroms. The gate was considered to be open when z-coordinate was less than -3.7 Angstroms. To determine the reported mean closed-gate currents for each applied bias, displacement of ions across each monomer was integrated across all periods characterized by a closed gate for that monomer. The slope of integrated displacement was taken for each of the four resulting traces and multiplied by ionic charge. A weighted average of the result, a set of four closed-gate current measurements, was taken to give the per-monomer mean current through the closed gate, a-b. The same process was used to find the per-monomer mean current through the open gate, c-d. The mean currents in Figure 3d-e were divided by 4 to give the per-monomer mean currents shown using dashed lines in panels a–d.



Movie S1: Animation illustrating a 40 ns simulation of the truncated AQP gating mechanism. The truncated AQP monomer is shown in green licorice, the Arg-197 gate in red licorice, and the lipid bilayer in orange lines. The crystallographic position of the Arg-197 gate is shown in translucent blue licorice. The direction of electric field from applied bias is indicated by the arrow, which changes color to emphasize changes in polarity. Na^+ is shown as yellow spheres, Cl^- as cyan spheres.



Movie S2: Animation illustrating a 960 ns simulation of the double-membrane truncated AQP ion pump. The movie consists of 26 still frames, each 38.4 ns apart, as the motion of ions makes an ordinary frame rate hard on the eyes. The truncated AQP tetramers are shown in cyan cartoon, the POPE lipid bilayer in brown lines and spheres, Na^+ in yellow spheres, and Cl^- in cyan spheres. The anode chamber, which loses the majority of its ions, is here depicted sandwiched between the two membranes.