



Figure 5.4. Pore formation and pore-mediated ion transport induced by a transmembrane imbalance of sodium ions. (A) 0 ps, the initial structure; (B) 1420 ps, appearance of a single water defect; (C) 1490 ps, redistribution of lipid headgroups toward the membrane interior; (D) 1710 ps, leakage of a sodium ion; (E) 2090 ps, leakage of a chloride ion; and (F) 10 ns, the metastable state of the water pore. Water is shown on the left- and right-hand sides of the figures, choline groups of lipid headgroups in dark, phosphate and glycerol groups using lighter color in the same region, and Na^+ (Cl^-) ions as light (dark) spheres. Nonpolar acyl chains of lipids are not shown. Excess of Na^+ ions is on the left-hand side. Reprinted with permission from [11]. Copyright © 2007, The Biophysical Society. The figure is adapted from (34).