

Water ordering at membrane interfaces controls fusion dynamics

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Supporting Information

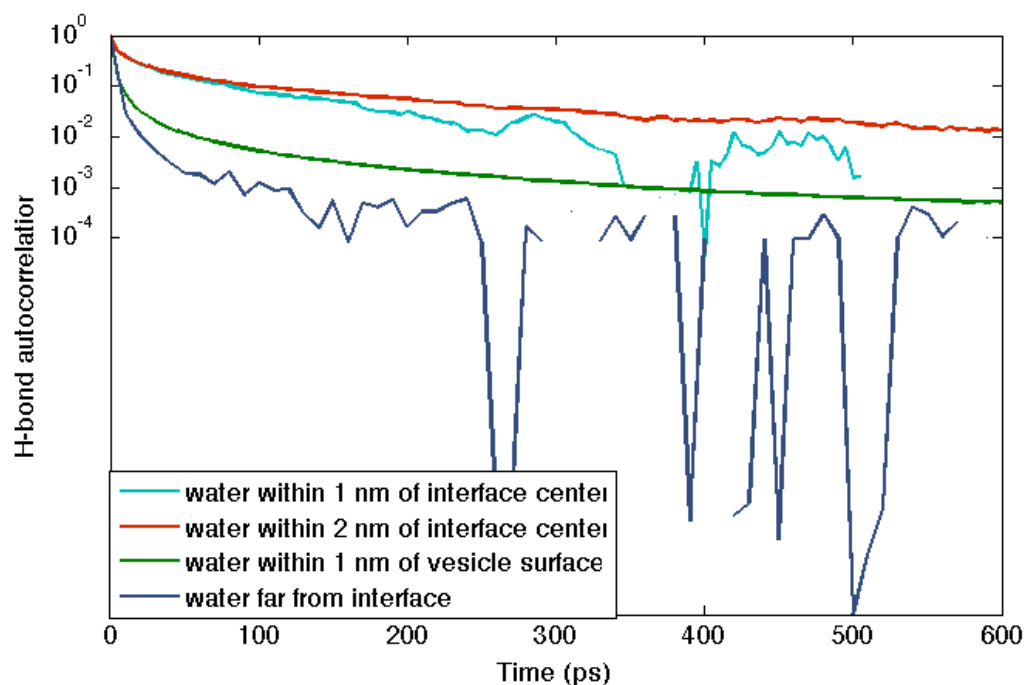


Figure S1. Slowed hydrogen-bond decorrelation near the vesicle-vesicle interface. Plotted are hydrogen bond autocorrelation times for water molecules within 1 nm of the vesicle surface but not within 2 nm of the interface center, water molecules within 2 nm of the vesicle-vesicle interface center, water molecules within 1 nm of the interface center, and water in a 4-nm cubic box not within 2 nm of any lipid molecule.

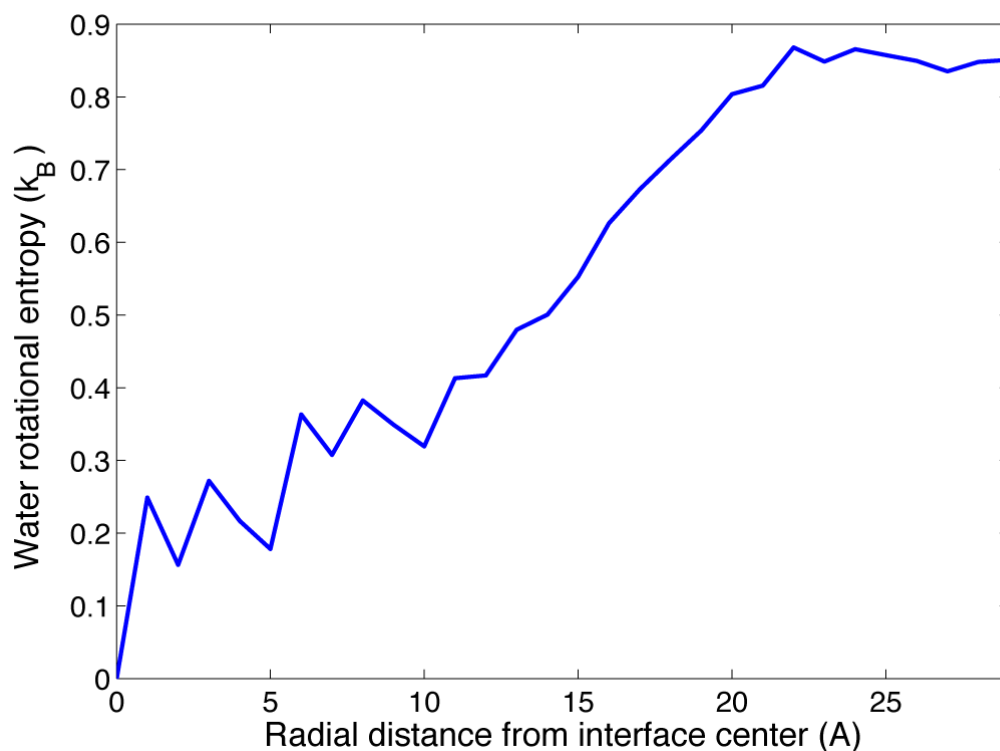


Figure S2. Decreased water rotational entropy near the vesicle-vesicle interface. Average water rotational entropy in units of k_B per $8\text{-}\text{\AA}^3$ voxel is plotted as a function of distance from a cylindrical axis defined by the two vesicle centers of mass and within a 2-nm-thick slice through the interface. Water rotational entropy is greatly decreased near the vesicle-vesicle interface center.

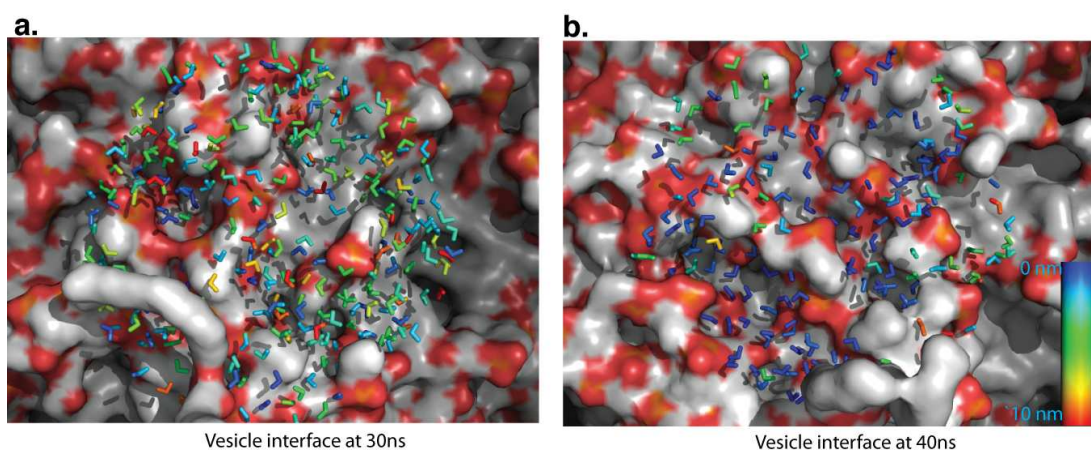


Figure S3. Decreased water mobility after formation of a vesicle-vesicle interface. Panels (a) and (b) show the distribution of water mobilities visually at 30 and 40 ns, with water molecules rendered in stick form against the surface of one vesicle and colored by displacement within a 1-ns interval. The 40-ns rendering is reproduced from Figure 1b for visual comparison.

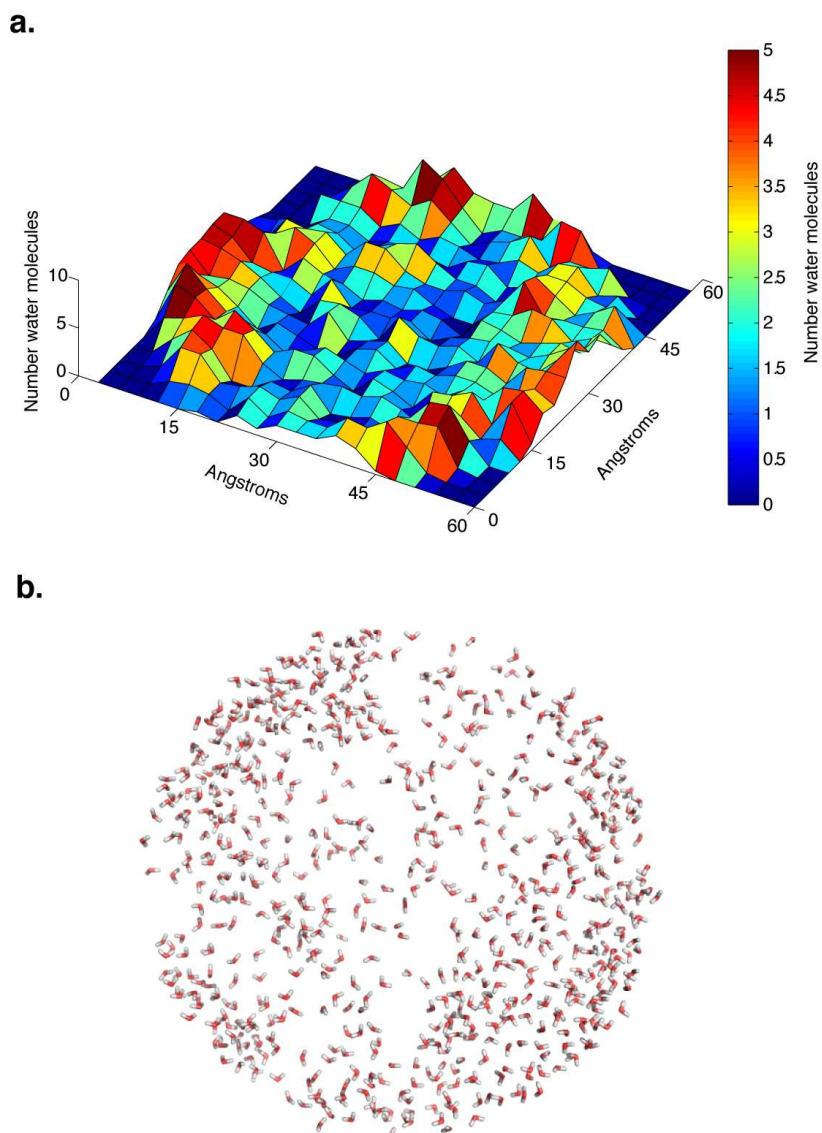


Figure S4. Patchy water structure at vesicle interface. Panel (a) shows the number of water molecules in a 20-Å slice through the vesicle-vesicle interface, calculated on a 3 Å x 3 Å grid. The slice is rendered directly in panel (b). The interfacial water displays a patchy structure but is typically 0-2 water molecules thick.

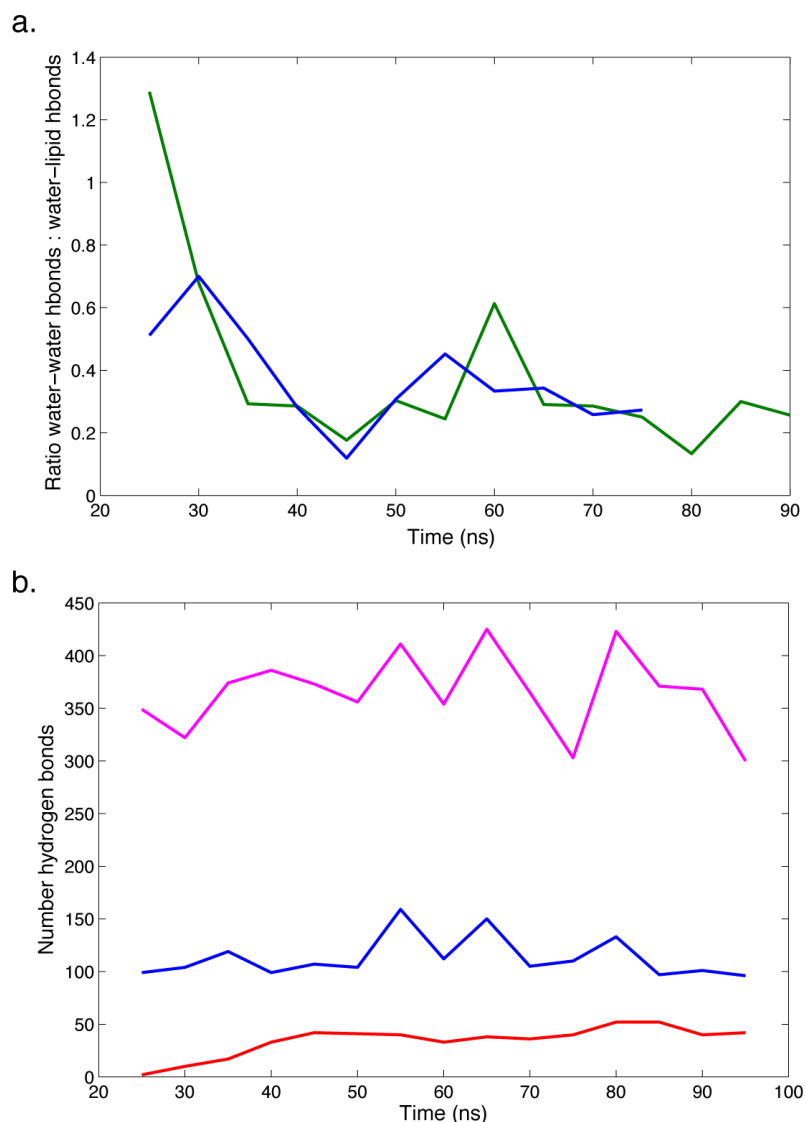


Figure S5. Ratio of water-water to water-lipid hydrogen bonds does not change substantially upon resolution. Panel (a) shows the ratio of water-water hydrogen bonds to water-lipid hydrogen bonds within 2 nm of the interface center, plotted in green for the original trajectory and in blue after resolution. The total number of hydrogen bonds in the interfacial region also does not change substantially upon resolution. Panel (b) shows the absolute number of hydrogen bonds in the original trajectory for water-water bonds in the interface (blue), water-lipid bonds in the interface (magenta), and inter-vesicle lipid-lipid bonds (red).