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Supporting Material

Atomistic simulations of “bicelle” mixtures

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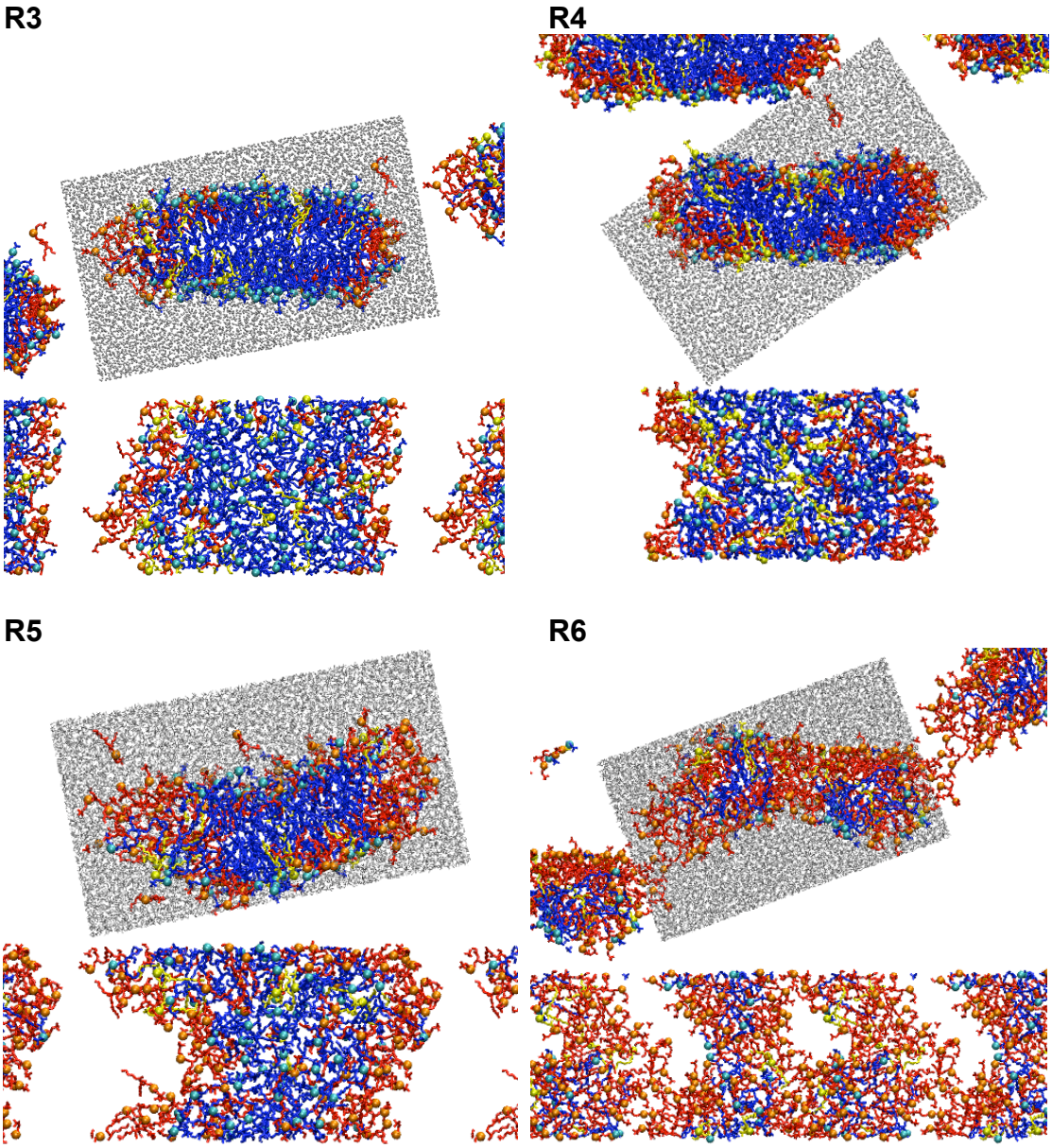

Figure S1: Snapshots of trajectory endpoints for ribbon simulations with increasing activity ratios α (trajectories R3-R6, viz. Table 2). Visualization is complicated by ribbon rotation about the ribbon edge (Z) axis. For each trajectory, the top image shows a view down the (Z) axis, with the simulation box positioned so the ribbon is roughly horizontal in the page, and solvent (gray) shown only for the primary simulation box to indicate the ribbon position in the periodic boundary scheme. Below each cross-sectional image is a "top-down" image generated by the rotating the top image 90° about the page horizontal direction. Blue, yellow, and red correspond to DMPC, DDPC, and DHPC respectively, with all phosphorus sites highlighted with spheres to indicate headgroup positions.

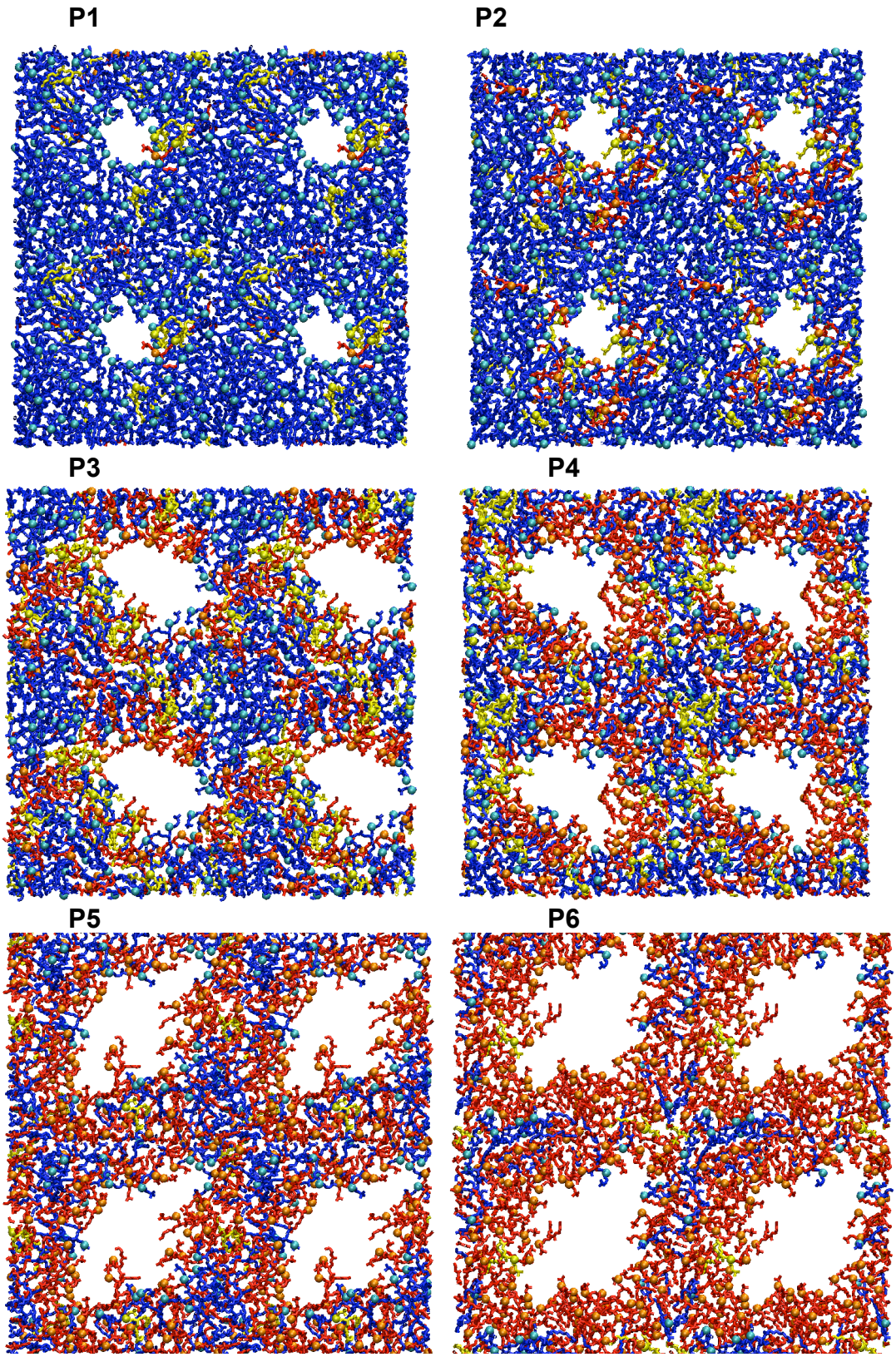

Figure S2: Trajectory endpoint snapshots of pores P1-P6 simulated at 300 K, showing 2×2 top-down view with solvent omitted. Simulation details are given in table 4. Blue, yellow, and red correspond to DMPC, DDPC, and DHPC respectively, with all phosphorus sites highlighted with spheres to indicate headgroup positions.

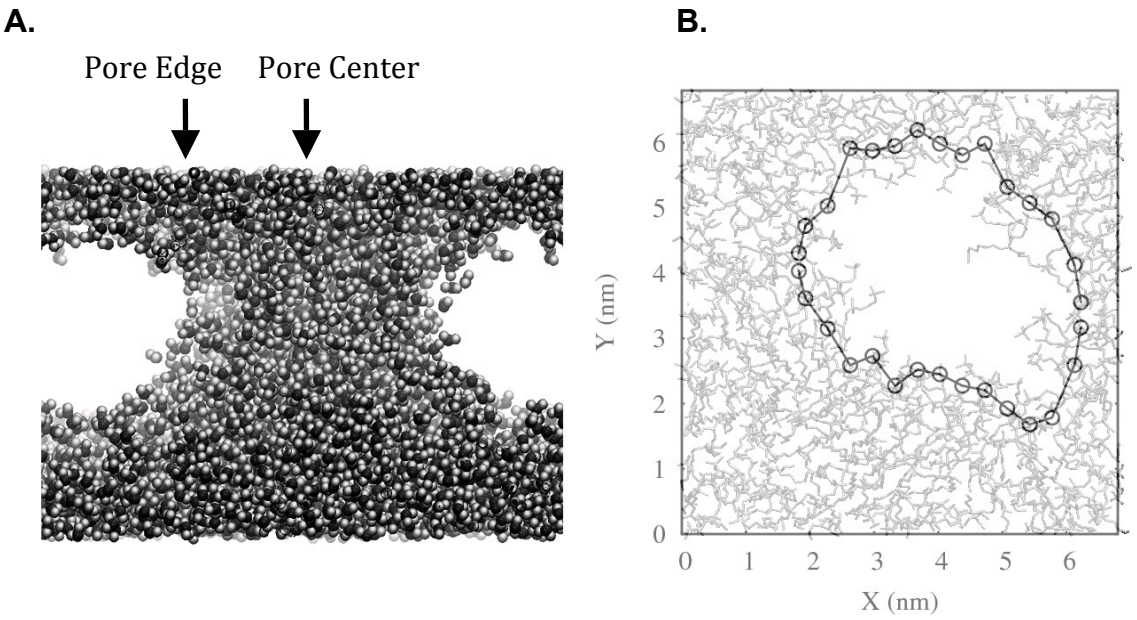

Figure S3. Illustration of the procedure used to determine the edge of a pore (a) and an example for the derived contour of a pore (b). Panel (a) shows a view of solvent molecules along the Y axis in the plane of the bilayer with lipids omitted for clarity (the white space). Water layer thickness is maximal in the center of the pore. The edge is defined where the water layer thickness drops to 70% of the maximum. Lipids within 1 nm from an edge point are considered to be at the edge. In (b), a top view, the lipids are represented by silver sticks and the edge of the pore is marked by open circles jointed by a solid line.

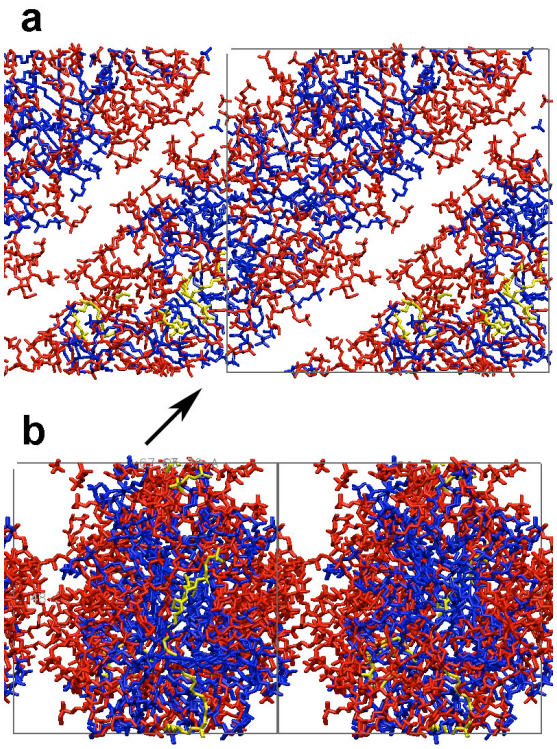

Figure S4. Top view (a) and lateral view (b) of endpoint of system P9 showing cylindrical micelle formed. Lateral view is taken along direction indicated by arrow. DMPC, DHPC and DDPC lipids are represented by blue, red and yellow sticks respectively. Grey lines denote the frame of the simulation box.