Supporting Information for

Membrane Remodeling by Surface-Bound Protein Aggregates: Insights From Coarse-Grained Molecular Dynamics Simulation

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The following figures represent results from a second simulation carried out under identical conditions as the one descried in main text, apart from differences the orientation of the protein molecules in the initial setup. Although the final aggregates in the two simulations somewhat differ in the overall shape and detailed bilayer interaction, their effect on the bilayer geometry and mechanical properties are similar.

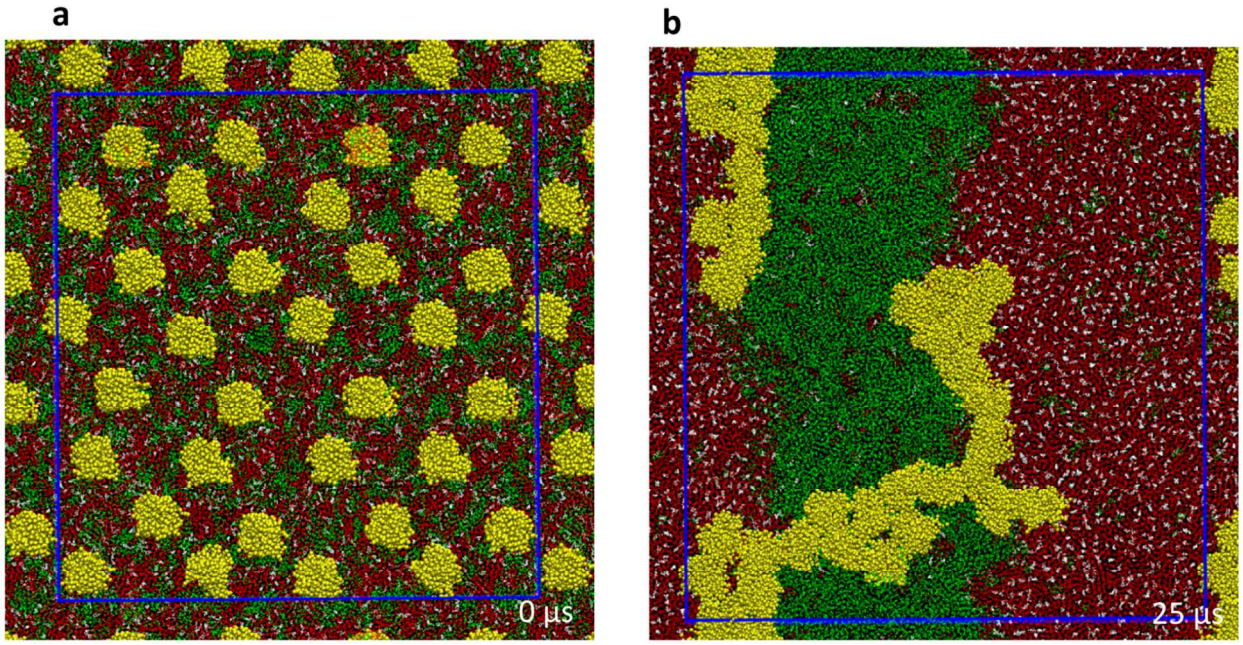

Figure S1. Snapshots from a CGMD simulation of a domain-forming bilayer with asymmetrically bound lipid-modified proteins: (a) the initial setup at 0 μs; (b) the final configurations at 25 μs. DPPC is shown in red, DLiPC in green, cholesterol in white and protein in yellow. Shown in blue is the actual simulation box, with the region outside being part of the periodic images in each direction.

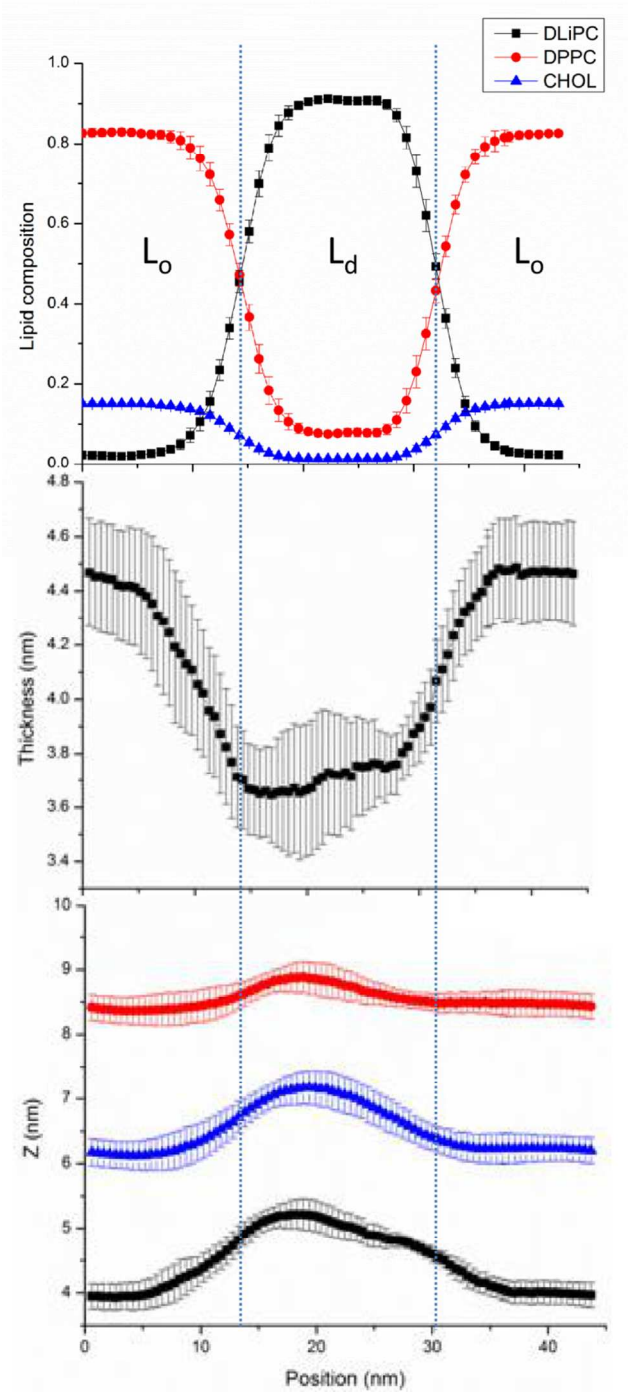

Figure S2. Lipid composition and geometry of the simulated bilayer. (a) The equilibrium lipid composition in the liquid ordered (L_o) and disordered (L_d) domains. Dotted lines demarcate the approximate domain boundary defined by the intersection point for the DLiPC and DPPC distributions. (b) Bilayer thickness calculated as the average distance between the PO4 beads at the two leaflets. (c) Average shape of the upper (red) and lower (black) monolayers and the mid-plane (blue) described by the average z-coordinate of the PO4 and the terminal acyl chain beads, respectively. In each panel, data represents average over the 16-25 μs portion of the trajectory; error bars were obtained by time block averaging

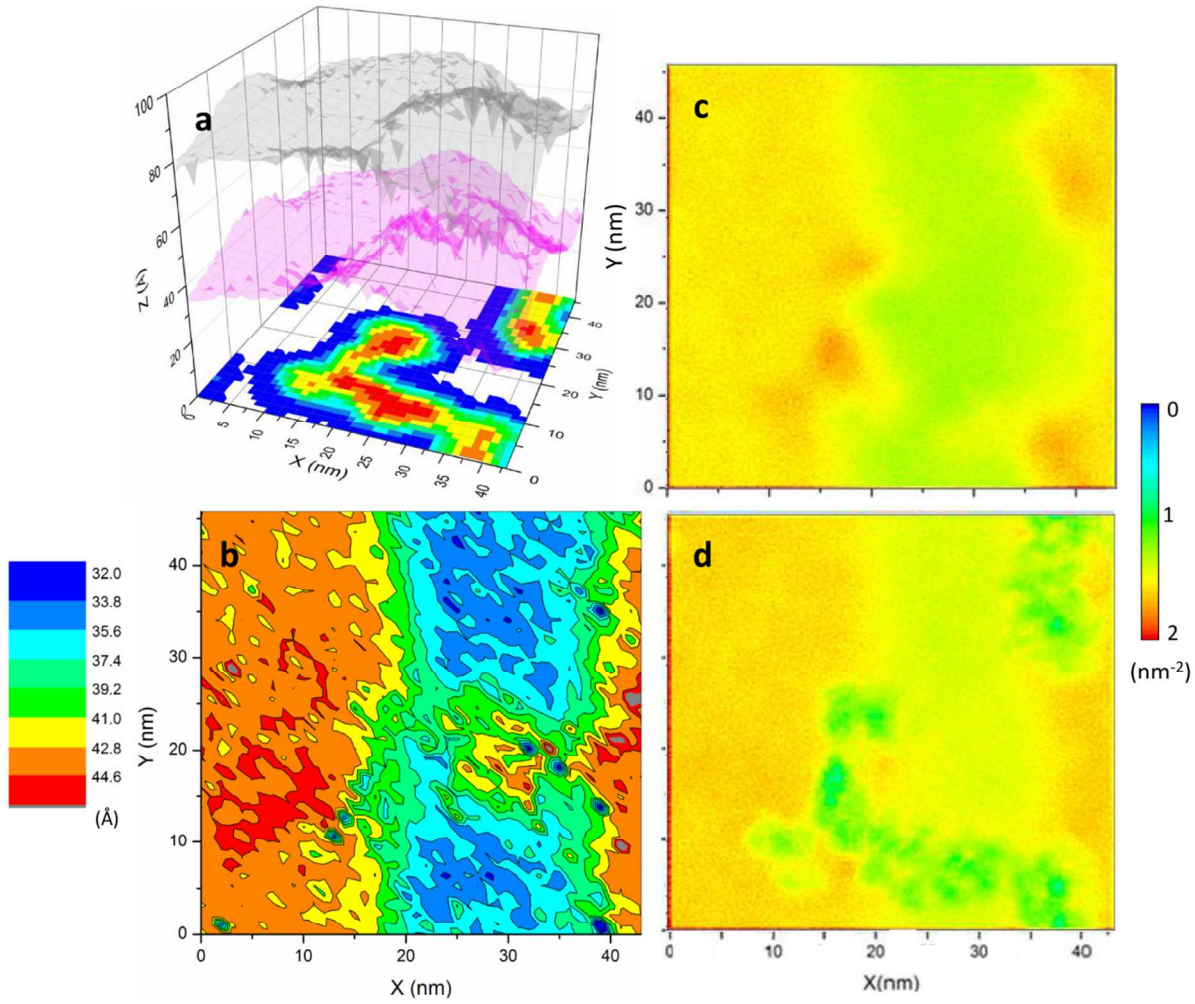

Figure S3. Variations in structure and composition across the bilayer surface (in the xy-plane). (a) The 3D shape of each monolayer and the location of the aggregate. The upper and lower leaflet, described by the average z-position of the PO4 beads, are in gray and magenta, respectively, whereas the normalized probability distribution of the protein is shown in heat map from high (red) to low (blue) density. (b) Change in thickness along the cross-section of the bilayer, measured by the average distance between the phosphate beads positions with each bin colored in red/orange for the L_o domain, blue/cyan for the L_d domain and green/yellow for the boundary between the two domains. (c-d) Lipid number density distribution at the upper (c) and lower (d) leaflets in blue (lowest density) through red (highest density).

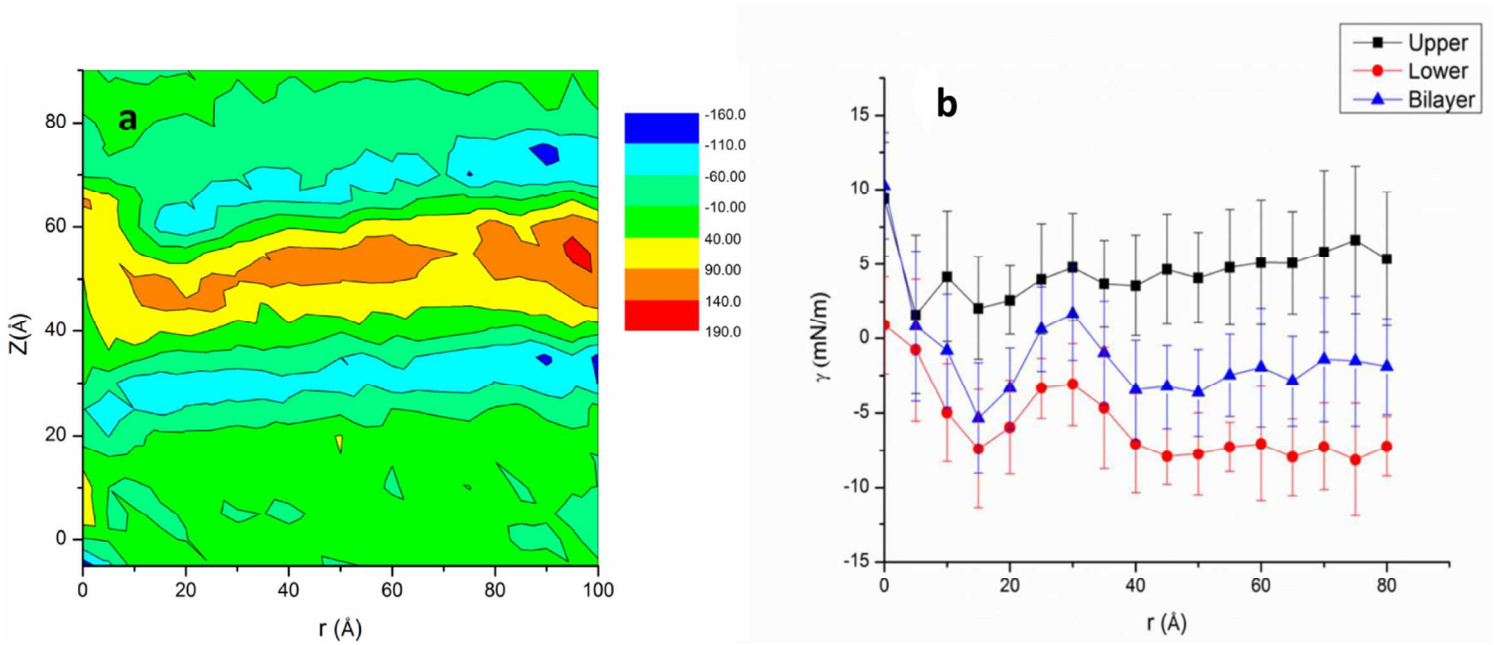

Figure S4. Lateral pressure profile and surface tension. (a) Lateral pressure profile π(z, r) as a function of the bilayer normal (z) and radial distance from the aggregate surface (r). (b) Time-averaged surface tension (γ) for each monolayer and the whole bilayer (errors bars from block averaging).