Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supporting Information

Simulation of Lipid Bilayer Self-Assembly using All-Atom Lipid Force Fields

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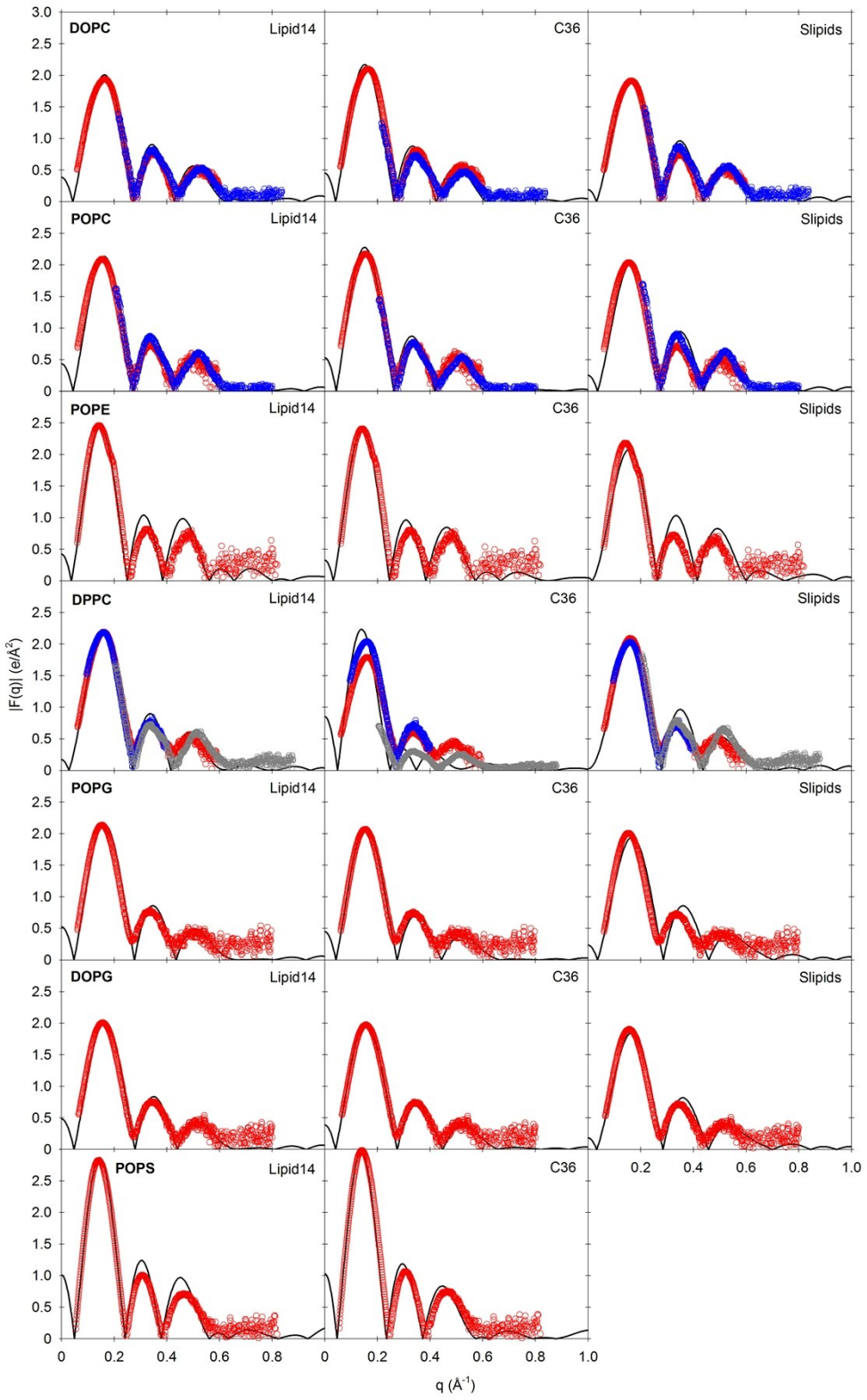
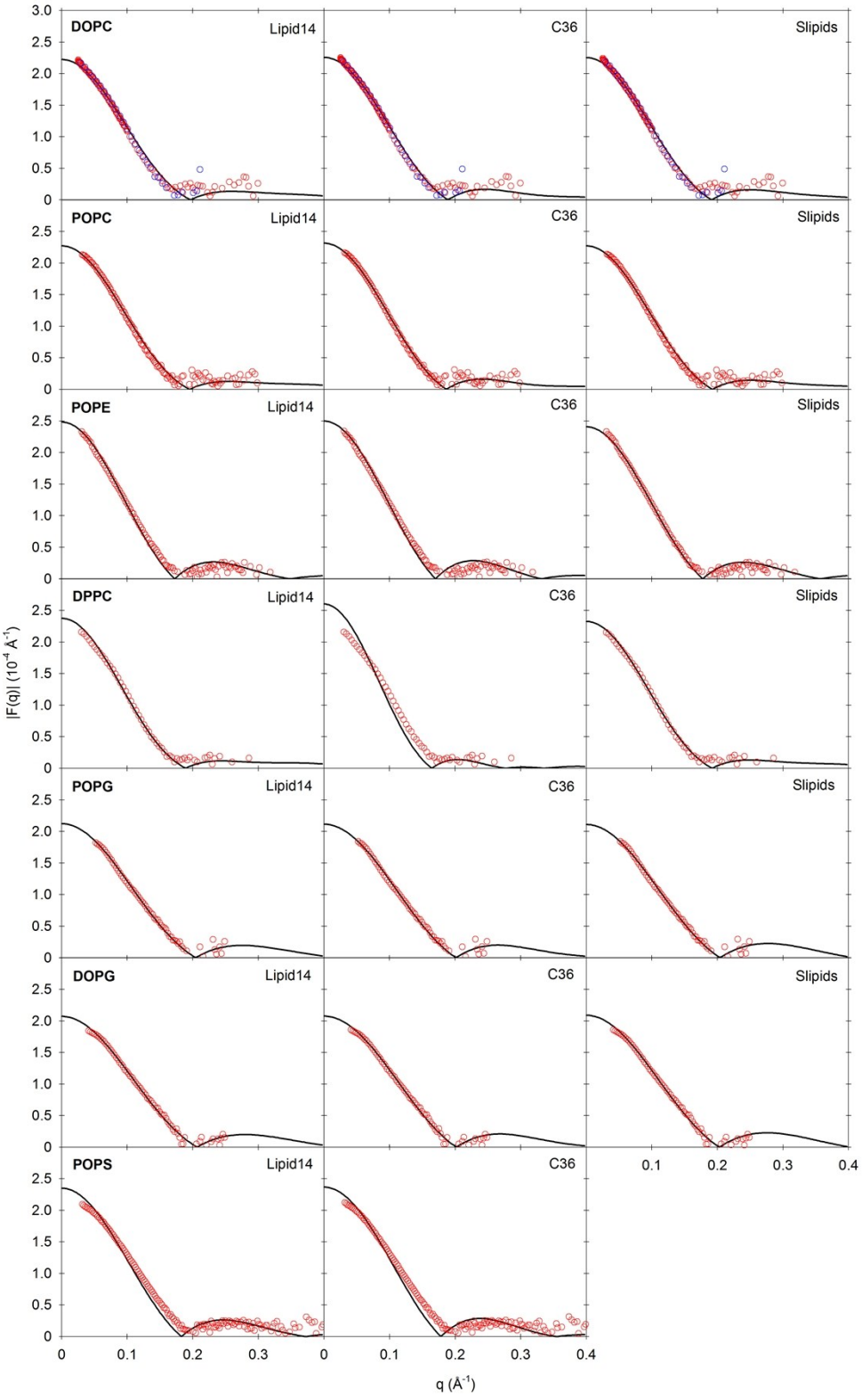
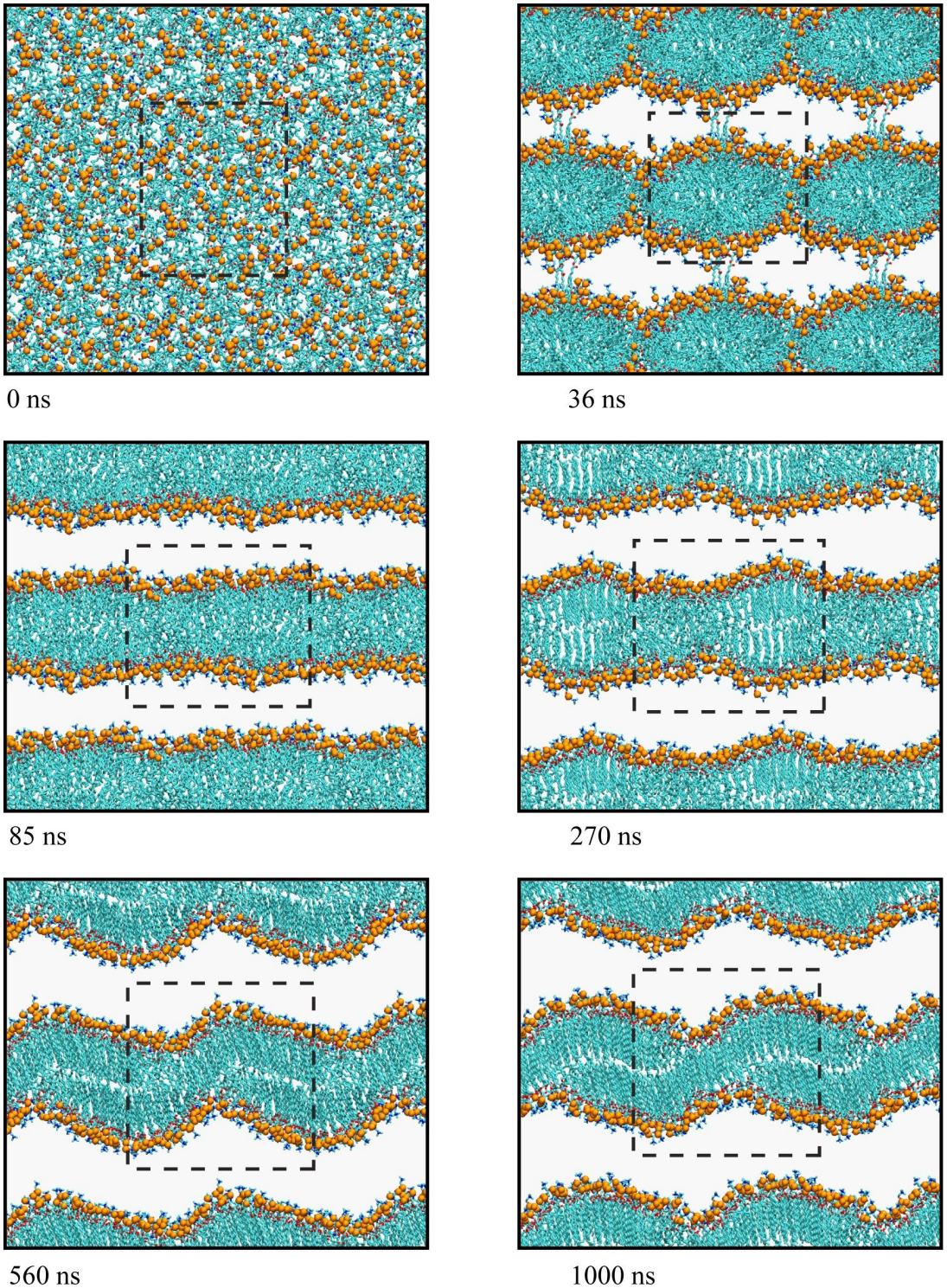
REFERENCES



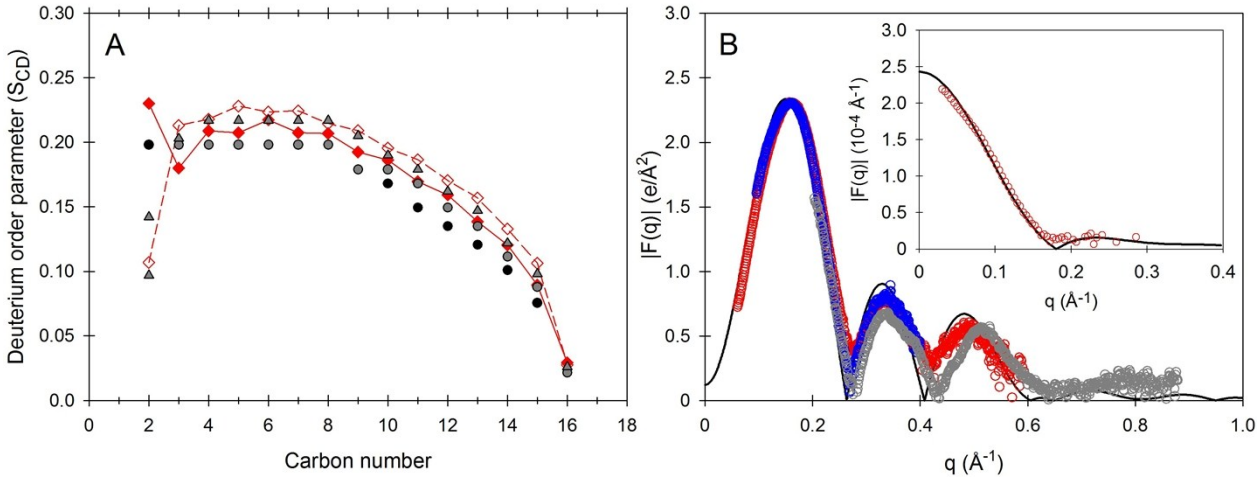
Supporting Figure 1. X-ray scattering form factors calculated for self-assembled bilayers (black line) and comparison with experiment (red, blue and gray circles)[1-7].



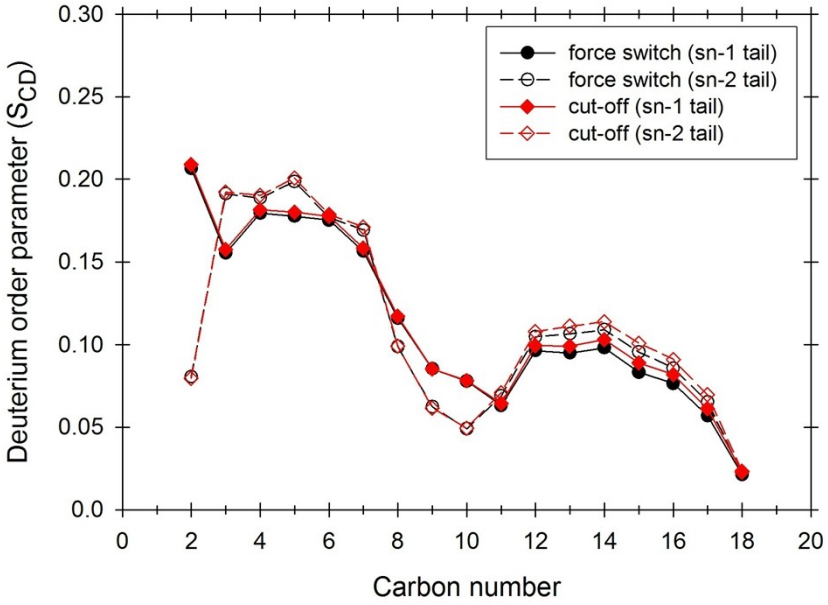
Supporting Figure 2. Neutron scattering form factors calculated for self-assembled bilayers (black line) and comparison with experiment (red and blue circles)[1, 2, 4-6, 8].



Supporting Figure 3. C36 DPPC self-assembly using a strict 10 Å cut-off. The snapshots are taken from the first simulation listed in Table 2a and are representative of all three repeats (though with different timings). The lipids eventually adopt a highly ordered configuration, where tails from opposite leaflets completely overlap in parts of the membrane (after 560, 600 and 700 ns for the three repeats, respectively). This configuration is very stable for the remainder of each simulation. The dashed-lined squares enclose the primary unit cell.



Supporting Figure 4. Deuterium order parameters (S_{CD}) and scattering form factors for self-assembled C36 DPPC bilayers in simulations run with a van der Waals force switch over 8 to 12 Å. Panel A: Simulation S_{CD} profiles were calculated as averages across all three repeats for the sn-1 (filled red diamonds and solid lines) and the sn-2 (open red diamonds and dashed lines) acyl chains. Experimental data[9, 10] are shown as black spheres for the sn-1 acyl chain and as gray spheres or upward triangles for the sn-2 acyl chain. Panel B: X-ray and neutron (inset) scattering form factors for the self-assembled bilayers (black lines) and comparison with experiment (red, blue and gray circles)[1, 2].



Supporting Figure 5. Comparison of deuterium order parameters (S_{CD}) for self-assembled C36 DOPC bilayers obtained with two different cut-off schemes. S_{CD} profiles calculated as averages across repeats performed with a van der Waals force switch over 8 to 12 Å are shown in black, and the profiles calculated from the original 10 Å cut-off simulations are shown in red (these are the same as in Figure 2).

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