Abstract Submitted
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Response of a self-assembling to mechanical stress[1] YVES DUBIEF, University of Vermont, Mechanical Engineering and Material Science Program, ROSS PACKARD, University of Vermont, Material Science program, SREEDHAR MANCHU, LEONIE COWLEY, University of Vermont, Mechanical Engineering Program — Coarse-grained molecular dynamics is used to characterize the mechanical properties of a solution of phospholipids and polyelectrolytes under shear and compression. DPPC (1,2-Dipalmitoylphosphatidylcholine), polyelectrolyes and water are coarse-grained using the MARTINI force field. Simulations are performed using both GROMACS and LAMMPS. In our simulation, the solution is confined by two rigid walls. The objective of this work is (i) to study influence of the electrostatic nature of the wall on the self-assembling structure of the solution and (ii) to define the rheological and structural response of the solution under shear and compression by moving one wall.

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