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Appendix

Table A1: Box lengths of the simulated bilayers for AA and CG simulations.

Model	System	x (nm)	y (nm)	z (nm)
AA	S1 (Maximum asymmetry)	10.38	10.38	9.02
	S2 (Maximum asymmetry)	12.77	16.91	8.97
	S3	12.70	17.07	8.95
	S4	15.71	15.12	8.16
	S5 (Intermediate asymmetry)	9.56	9.56	10.64
	S7 (Minimum asymmetry)	14.05	15.81	8.72
	S8 (Minimum asymmetry)	13.68	15.51	9.15
CG	S1 (Maximum asymmetry)	10.43	10.43	8.66
	S2 (Maximum Asymmetry)	13.43	17.80	7.97
	S3	13.12	17.62	8.15
	S4	15.85	15.25	7.75
	S5 (Intermediate asymmetry)	9.54	9.54	10.42
	S6 (Intermediate asymmetry	28.6	28.6	10.37
	S7 (Minimum Asymmetry)	14.70	16.54	7.74
	S8 (Minimum asymmetry)	14.33	16.24	8.15

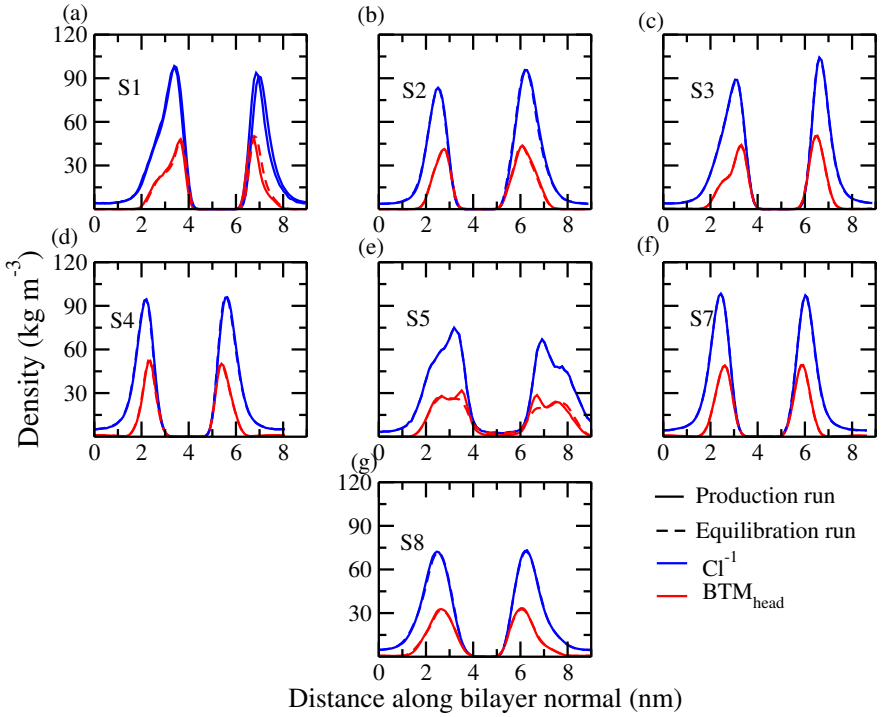

Figure A1: Density distributions of chloride ions and BTMAC head-groups obtained from AA simulation for equilibration and production runs. The ions reside near the BTMAC heads via electrostatic interactions and thus the location of ions do not change for both the run-lengths.

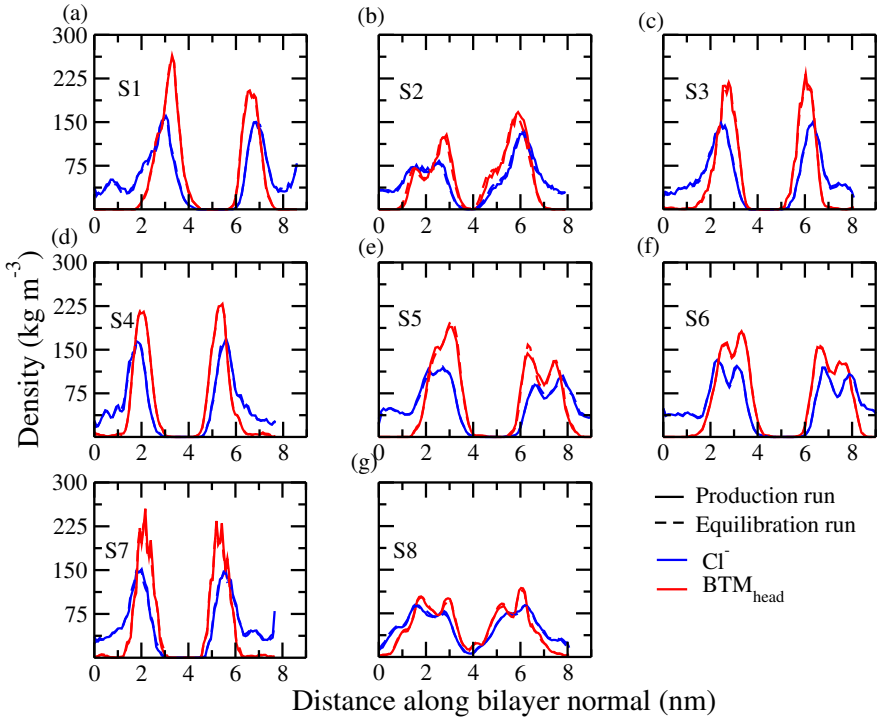

Figure A2: Density distributions of chloride ions and BTMAC head-groups obtained from CG simulation for equilibration and production runs. The ions stay closer to the BTMAC heads via electrostatic interactions and thus the location of ions do not change for both the run-lengths.

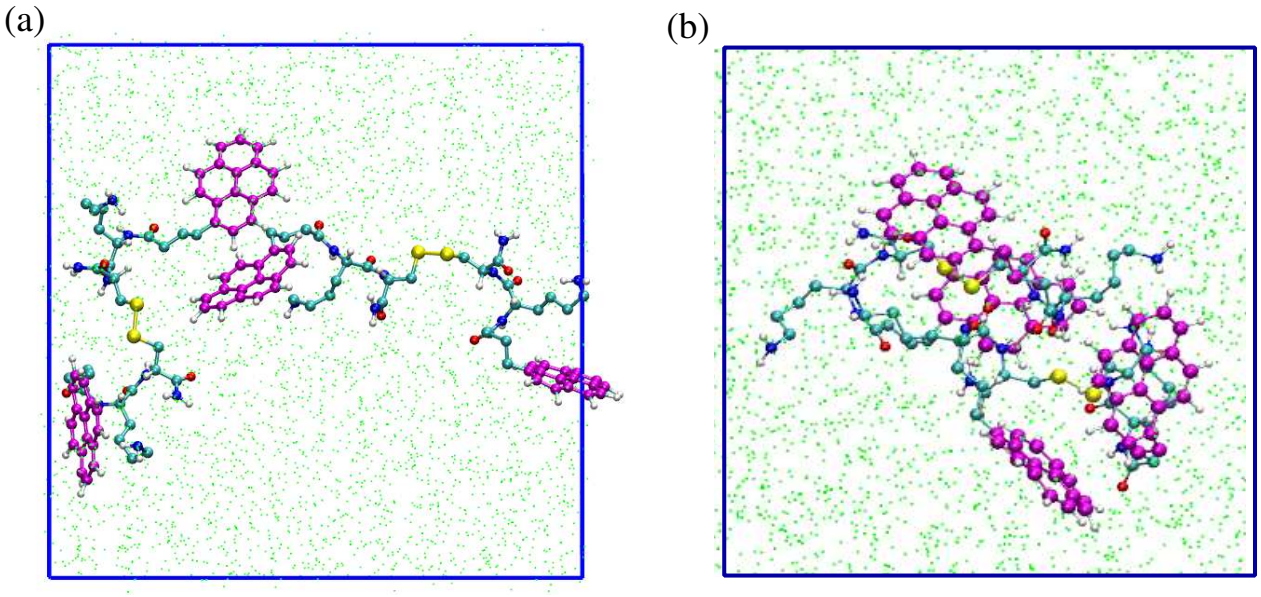

Figure A3: (a) Initial and (b) final snapshot of two open PyKC dimers. The open chain dimers adopt a folded conformation after simulation in an NPT ensemble.