

Supporting Information

Interaction of antimicrobial lipopeptides with bacterial lipid bilayers

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Numerical values

Table S1: Numerical values of properties of interest.

System	POPE- A_L (\AA^2)	POPG- A_L (\AA^2)	d_{HH} (\AA)	k_A (dyn/cm)	P_W ($\mu\text{m/s}$)
Bacterial	56.6 ± 0.2	63.1 ± 0.2	41.3 ± 0.4	219.5 ± 14.0	19.8
10% AMLP	54.8 ± 0.1	60.9 ± 0.4	41.6 ± 0.2	239.5 ± 20.4	15
25% AMLP	55.1 ± 0.3	61.5 ± 0.2	39.4 ± 0.2	240.6 ± 28.8	24.6
40% AMLP	59.4 ± 0.6	62.1 ± 0.6	34.1 ± 0.13	128.2 ± 4.6	54

Electron density profiles

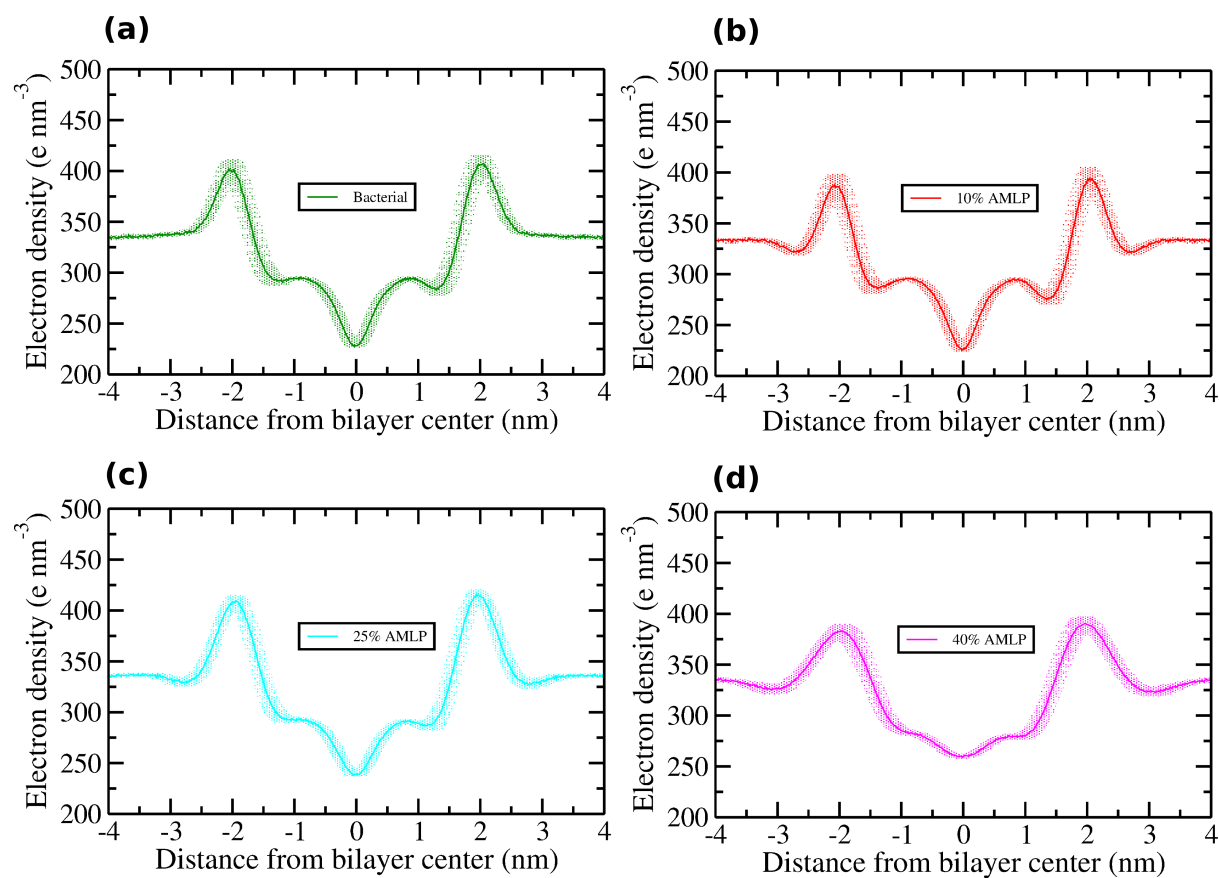


Figure S1: Electron density profiles with error bars for (a) bacterial, (b) 10% AMLP, (c) 25% AMLP and (d) 40% AMLP systems.

Phosphate electron density profiles

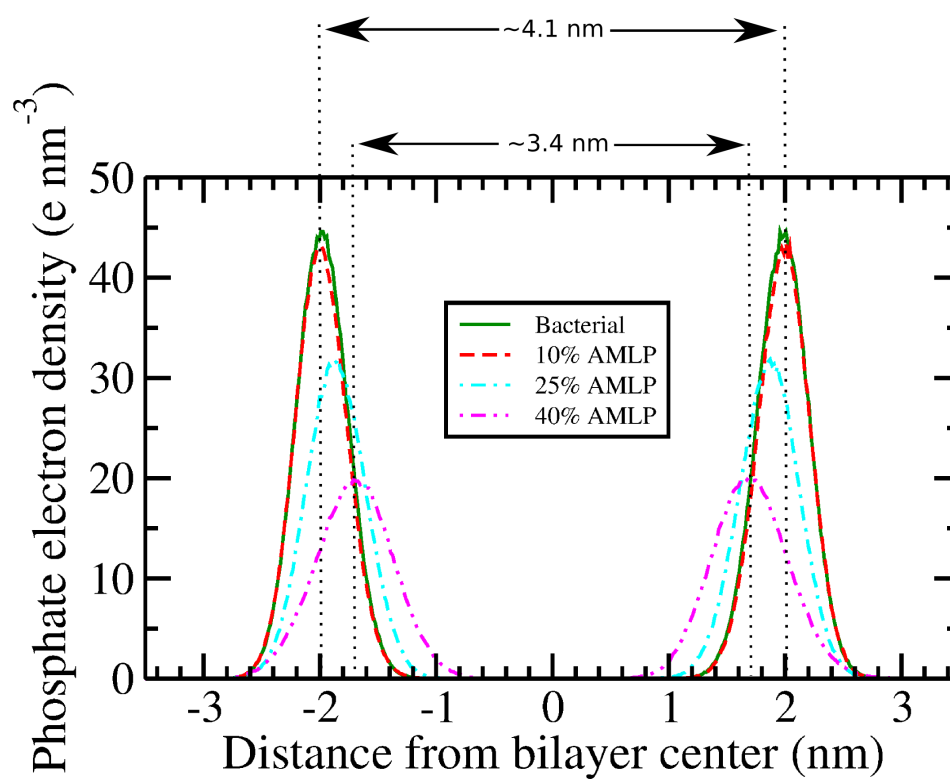


Figure S2: Electron density profiles for phosphate atoms in all four simulated systems. The peaks here better highlight the differences in their bilayer thicknesses.

Interdigitation of lipid chains

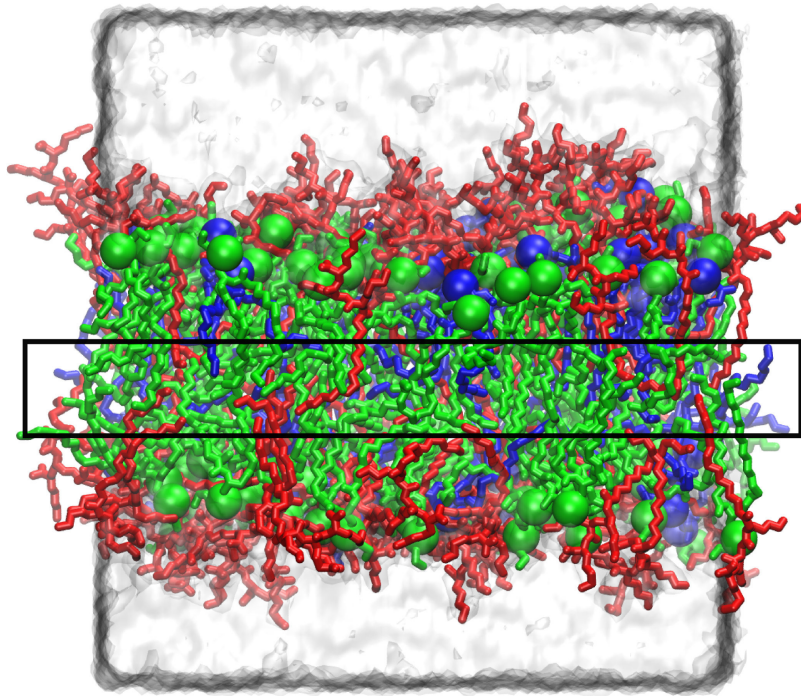


Figure S3: Lipid chain interdigitation as seen in the bilayer core of the 40% AMLP system. The PEs are coloured green, PGs are blue and AMLPs are red.

Water permeation

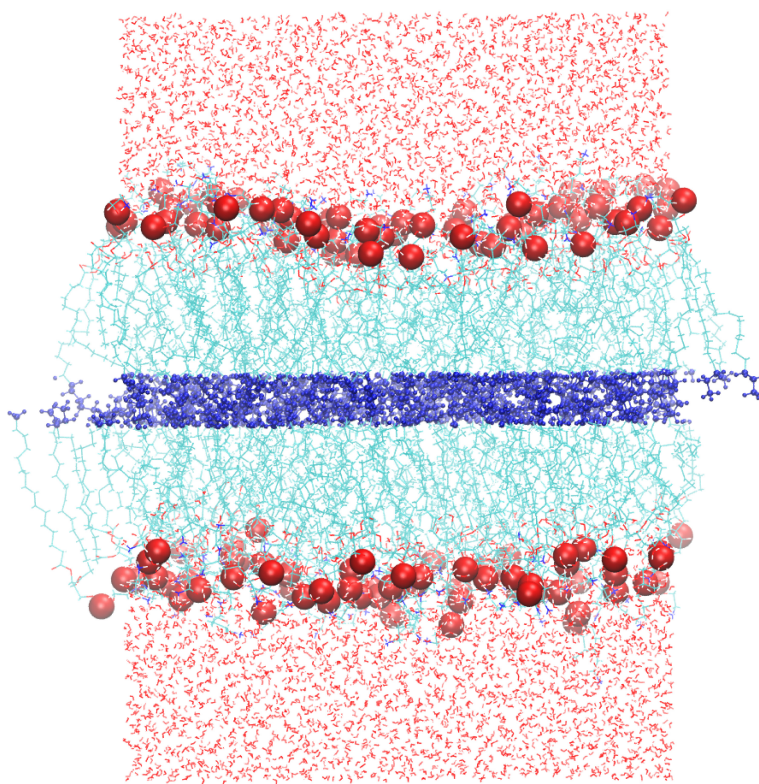


Figure S4: Central region of bilayer core defined for water permeation calculations as shown using the CPK representation and coloured in dark blue.

Lateral pressure profiles

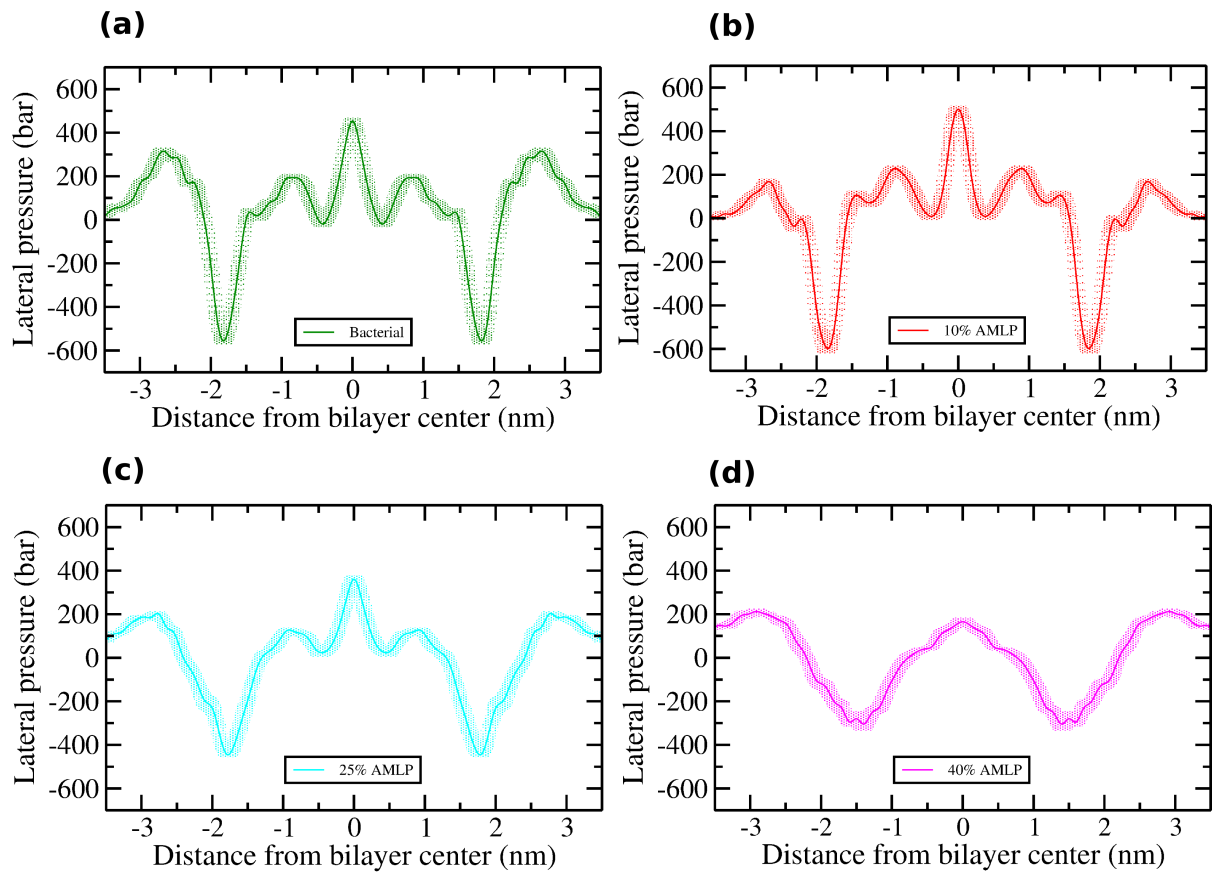


Figure S5: Lateral pressure profiles with error bars for (a) bacterial, (b) 10% AMLP, (c) 25% AMLP and (d) 40% AMLP systems.

Dipole potential profiles

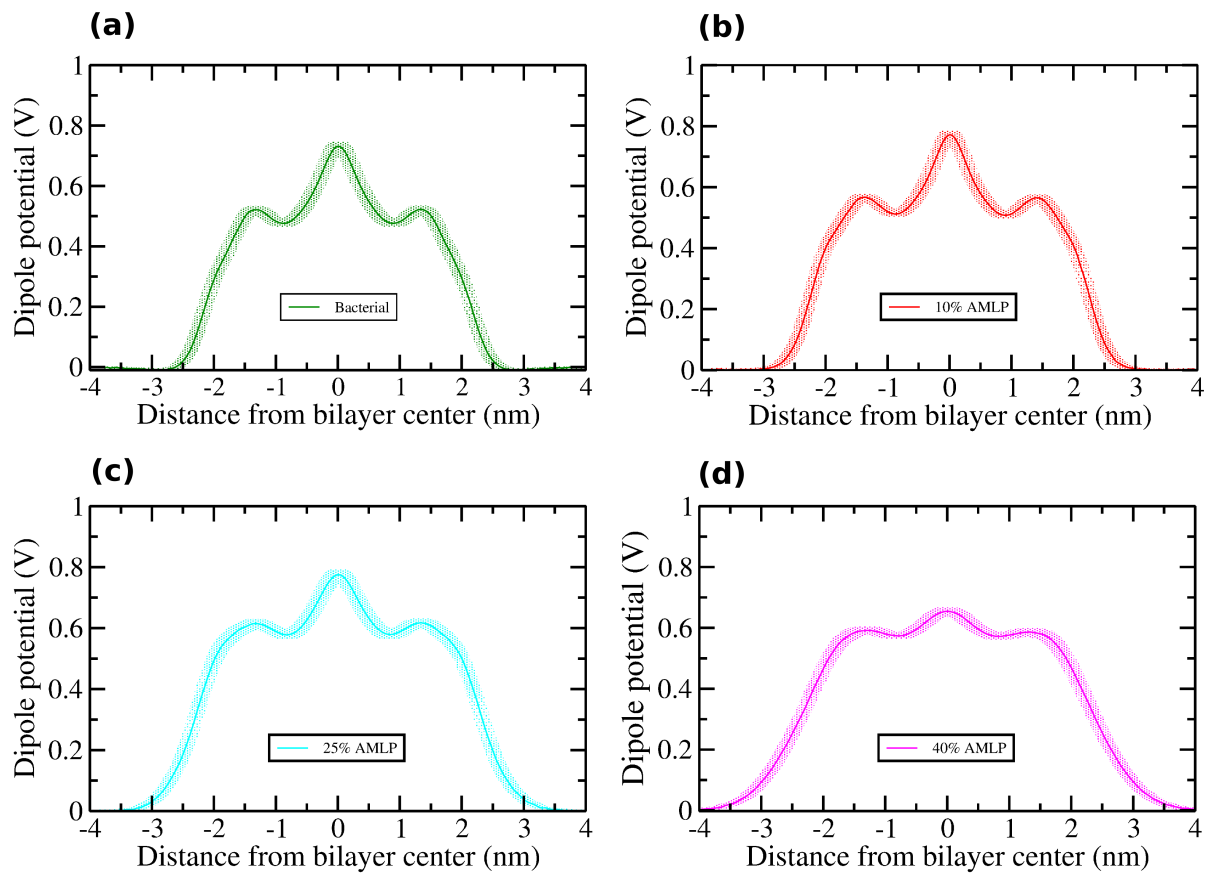


Figure S6: Dipole potential profiles with error bars for (a) bacterial, (b) 10% AMLP, (c) 25% AMLP and (d) 40% AMLP systems.

Dipole potential contributions

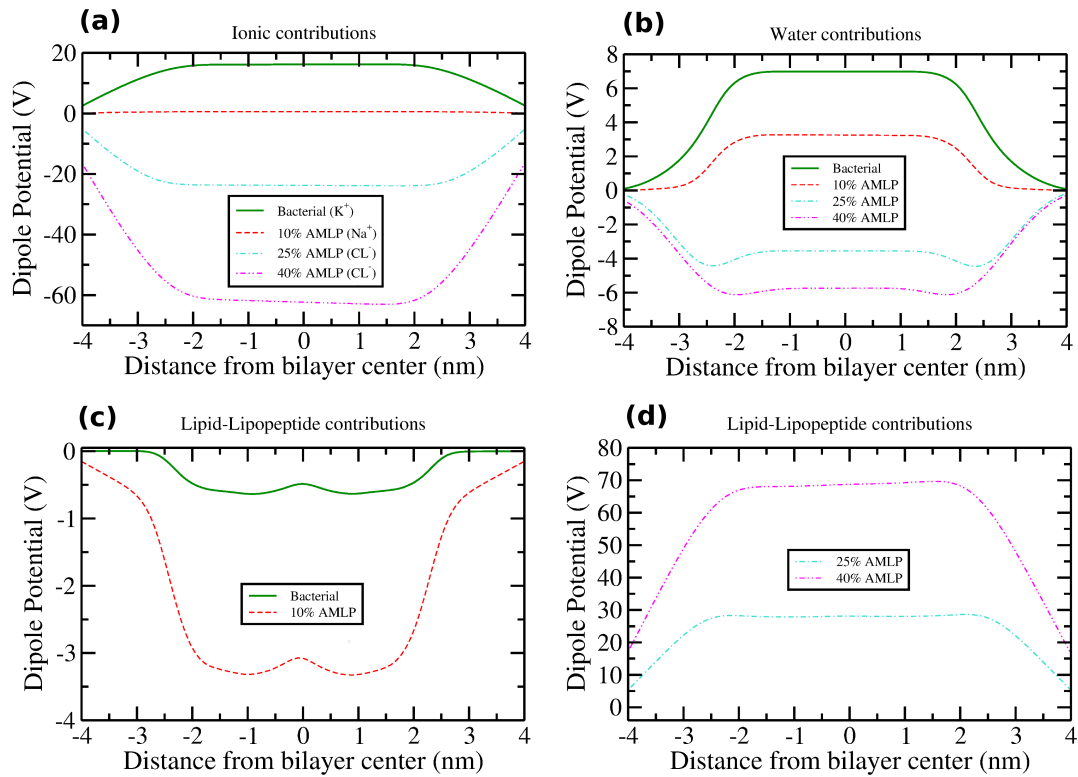


Figure S7: Individual contributions of the dipole potential profile from (a) ions, (b) water and (c-d) lipids-lipopeptides. For all systems, the net positive dipole potential comes from a sum total of larger positive and negative contributions, which come from different components in different systems. For the bacterial and "10% AMLP" systems the net positive contributions come from water and ions while the negative ones come from lipid and lipopeptides. On the other hand, the positive contributions come from lipids and lipopeptides for the 25 and 40 mol% AMLP systems, while the negative ones come from water and ions.