Supporting Information

Membrane Binding of Peptide Models for early Stages of Amyloid Formation: Lipid Packing Counts more than Charge

Maria Hoernke[124], Stephanie Tassler[1], Beate Koksch[3], Gerald Brezesinski[14]

5.1. Interaction the Peptides i,i+2 and i,i+4 with Layers of DPPC or DPPG

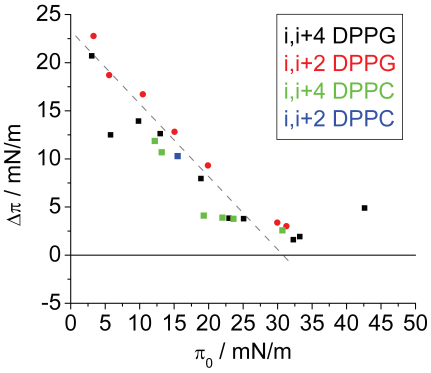
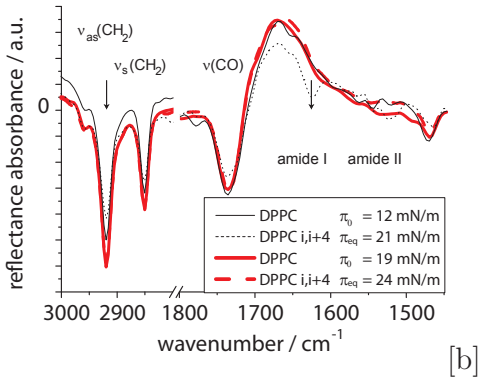


Figure S 1: Comparison of equilibrium pressures π_{eq} versus initial surface pressure π_0 for bot peptides i,i+2 and i,i+4 and DPPC as well as DPPG monolayers. (0.3 μM i,i+4 or i,i+2 respectively, 10 mM PBS, pH 7.4, 150 mM NaCl, 20 °C, preformed DPPC or DPPG spread from $CHCl_3$ to yield the corresponding π_0)

5.2. IRRA Spectra of i,i+4 Adsorbed to DPPC

[1]Max Planck Institute of Colloids and Interfaces, Golm, 14424 Potsdam, Germany
[2]currently: Centre for Biological Signalling Studies, Albert-Ludwigs-Universitt, Hermann-Herder-Str. 9, 79109 Freiburg i.Br., Germany
[4]corresponding authors: maria.hoernke@bioss.uni-freiburg.de, brezesinski@mpikg.mpg.de
[3]Institute of Chemistry and Biochemistry, Freie Universitt, Takustr.3, 14195 Berlin, Germany



[b]

Figure S 2: IRRA spectra of pure DPPC monolayers (solid lines) and DPPC after adsorption of i,i+4 reaches equilibrium (broken lines) at various π. Two cases are presented, first for $\pi_0 \approx \pi_{LE-LC}$ and second for $\pi_0 > \pi_{LE-LC}$ (thick grey lines). The spectra are chosen so that π_{eq} corresponding to the black broken curve is close to π_0 corresponding to the solid grey line. Arrows are guides for the eye, illustrating the change in the spectra upon increasing π or adsorption of i,i+4, respectively. (0.3 μM i,i+4, 10 mM PBS, pH 7.4, 150 mM NaCl, 20 °C, preformed DPPC spread from $CHCl_3$ to yield the corresponding π_0, p-polarized light, angle of incidence: 40°)

5.3. Lipid Packing Parameters

Upon compression, the peak patterns of both types of lipid layers change characteristically. First, the q_z value of the peaks at large q_z decreases. This is the result of decreased chain tilt. Second, the q_{xy} values of all peaks increase slightly. Thereby, the shift of peaks at higher q_z is larger than for those at small q_z. These changes correspond to smaller dimensions of the unit cell, i.e., a contraction of the unit cell accompanied by a decrease in tilt angle. Third, due to the rearrangement within the film, the correlation length may change.

5.4. SAXS of DMPG: diffuse scattering and metastable states

Different from DMPC, the anionic lipid DMPG is usually forming vesicles of uncorrelated bilayers, instead of stacked bilayers. Therefore, the main feature of SAXS data is the correlation peak corresponding to the electron density profile of single bilayers. Data analysis is further complicated by the sensitivity of DMPG dispersions on temperature treatment.

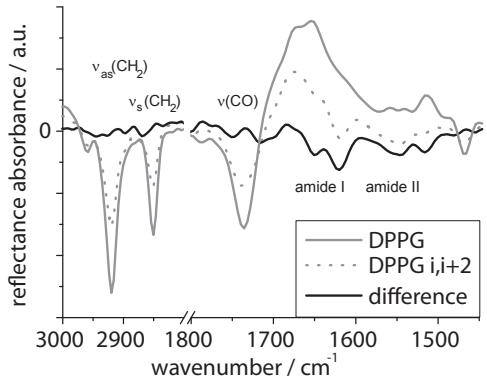


Figure S 3: IRRA spectra of the pure DPPG layer, the DPPG layer interacting with i,i+2 after 24 h hours of adsorption and difference spectrum. π_{eq} = 24 mN/m (0.3 μM i,i+2, 10 mM PBS, pH 7.4, 150 mM NaCl, 20 °C, preformed DPPG spread from $CHCl_3$ to yield the corresponding π_0)

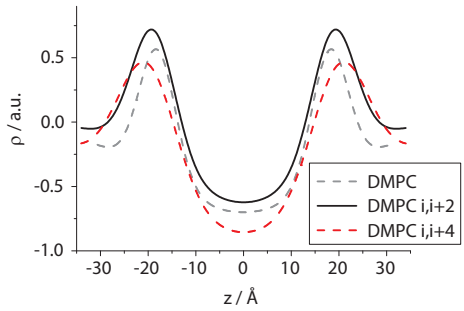


Figure S 4: SAXS: Electron density profiles of DMPC, DMPC with i,i+2 and i,i+4, respectively. (5 °C, 10 mM PBS, 150 mM NaCl, pH 7.4) Fits were obtained using GAP.

Table 1: GIXD analysis of DPPC films at 20 °C. The distortion (dist.) denotes the type of acyl chain packing being either oblique (obl) or orthorhombic with distortion direction and tilt direction to the next neighbour (NN). a and b are the dimensions of the unit cell and γ is the angle between these two vectors. t t denotes the tilt angle to the surface normal and A_0 is the cross-sectional area of one acyl chain.

sample errors	q_{xy} / Å^{-1}	q_z / Å^{-1}	L_{corr} / Å ± 20 Å	dist.	a / Å ± 0.05 Å	b / Å	γ / ° ± 1°	t / ° ± 1°	A_0 / Å^2 ± 0.2 Å^2
DPPC									
15 mN/m	1.458	0.087	500	obl	5.16	5.22	112.3	36	20.2
	1.317	0.787	110						
	1.300	0.790	120						
25 mN/m	1.465	0.0	540	obl	5.09	5.17	113.6	32	20.3
	1.348	0.647	180						
	1.327	0.765	110						
30 mN/m	1.468	0.082	510	obl	5.04	5.15	114.4	30	20.5
	1.368	0.582	150						
	1.340	0.710	95						
40 mN/m	1.474	0.0	215	obl	4.99	5.03	116.6	25	20.4
	1.408	0.426	135						
	1.397	0.610	80						
DPPC i,i+4									
30 mN/m	1.466	0.0	300	NN	5.50	5.09	122.6	31	20.1
	1.360	0.690	70						
40 mN/m	1.472	0.0	340	NN	5.35	5.04	122.1	26	20.4
	1.385	0.586	80						

Table 2: GIXD analysis of DPPG films at 20 °C. The distortion (dist.) denotes the type of acyl chain packing being oblique (obl) in all cases. a and b are the dimensions of the unit cell and γ is the angle between these two vectors. t denotes the tilt angle to the surface normal and A_0 is the cross-sectional area of one acyl chain.

sample errors	q_{xy} / Å^{-1}	q_z / Å^{-1}	L_{corr} / Å ± 20 Å	dist.	a / Å ± 0.05 Å	b / Å	γ / ° ± 1°	t / ° ± 1°	A_0 / Å^2 ± 0.2 Å^2
DPPG									
20 mN/m	1.46	0.088	475	obl	5.12	5.23	112.6	37	19.9
	1.330	0.720	110						
	1.301	0.870	200						
30 mN/m	1.470	0.083	420	obl	5.03	5.14	114.8	31	20.0
	1.377	0.600	105						
	1.347	0.730	140						
40 mN/m	1.470	0.083	360	obl	4.99	5.07	116.2	27	20.2
	1.404	0.570	130						
	1.380	0.630	240						
DPPG i,i+4									
20 mN/m	1.466	0.0	575	obl	5.05	5.17	114.0	36	19.4
	1.3632	0.683	130						
	1.332	0.893	180						
30 mN/m	1.472	0.080	580	obl	4.98	5.10	116.1	28	19.9
	1.406	0.590	170						
	1.377	0.673	160						
40 mN/m	1.481	> 0	480	obl	4.93	5.00	117.3	23	20.2
	1.435	0.480	140						
	1.411	0.530	370						

Table 3: Parameters obtained from the best fit of the SAXS data. DMPC 5 °C. d: d-spacing, N_{corr}: average number of correlated bilayers, $N_{single/multi}$: ratio of uncorrelated to correlated bilayers, z_{hg}: position of the head group Gaussian from the centre of the bilayer, σ_{hg} and σ_{chains}: FWHM values of the head group and chain Gaussian, respectively, ρ_{chains}: electron density of the chains with respect to the head group layer.

sample	d / Å	N_{corr}	z_{hg} / Å	σ_{hg} / Å	σ_{chains} / Å	ρ_{chains}	$N_{single/multi}$	d_b / Å
errors	± 1 Å	± 2	± 0.05 Å	± 0.2 Å	± 0.7 Å	± 0.05		± 1.5 Å
DMPC	61.3	11.7	18.06	3.8	18.6	-0.70	0.77	51.3
DMPC i,i+2	-	-	18.85	4.5	15.1	-0.62	1.0	55.8
DMPC i,i+4	68.1	11.5	20.14	5.9	21.0	-0.86	>0.99	64.2