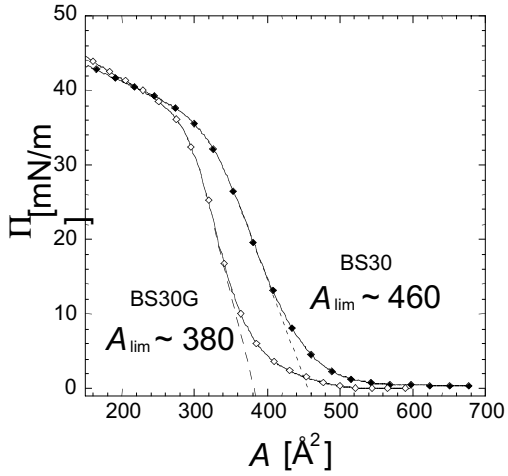
Supporting information

Assembly of triple-stranded β-sheet peptides at interfaces

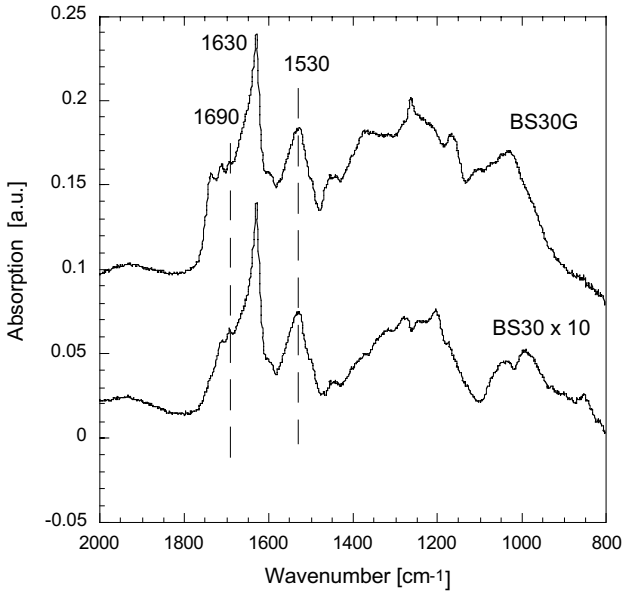
Hanna Rapaport[1], Gunter Möller[2], Charles M. Knobler[2], Torben R. Jensen[3], Kristian Kjaer[3], Leslie Leiserowitz[4] and David A. Tirrell[1]

[1]*Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, California 91125, USA*
[2]*Department of Chemistry and Biochemistry, University of California, Los Angeles, CA 90024-1569 USA*
[3]*Materials Research Department, Risø National Laboratory, DK-4000 Roskilde, Denmark*
[4]*Department of Materials and Interfaces, Weizmann Institute of Science, Rehovot 76100, Israel*

1. Surface pressure-molecular area isotherms of BS30 and BS30G

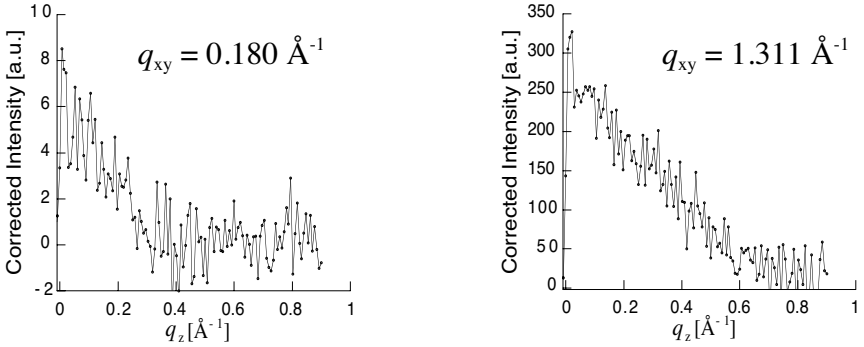


2. ATR-FTIR absorption spectra of BS30 and BS30G Langmuir films transferred to ZnSe ATR prisms



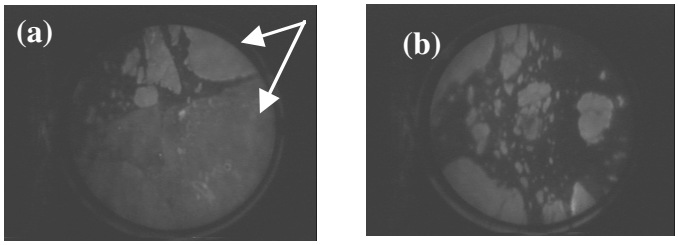
Langmuir films of the peptides BS30 and BS30G (each at a nominal area per molecule of ~ 370 $Å^2$/molecule corresponding to an average of a 1.5 monolayer thick film coverage) were transferred from the air-water interface to a ZnSe prism by horizontal deposition. Both BS30 and BS30G spectra exhibit amide I absorption bands at 1630 cm^{-1} and at 1695 cm^{-1}, characteristic of anti-parallel β-sheet structures. The amide II band, at ~1515-1520 cm^{-1}, characteristic of pleated β-sheets, is present in the spectra of BS30 and BS30G but slightly shifted to 1530 cm^{-1}. The ATR-FTIR absorption spectra of BS30 and BS30G exhibit no distinct differences, consistent with the β-sheet structure.

3. Grazing incidence X-ray diffraction-Bragg rods



The crystalline coherence length L_{xy} may be calculated from the Scherrer formula (see reference 4): $L_{xy} = 0.9(2\pi) / \text{FWHM}(q_{xy})$. Similarly, the width of the Bragg rod profile along q_z, FWHM(q_z) gives an estimate of the thickness of the crystalline film as $L_z \approx 0.9(2\pi) / \text{FWHM}(q_z)$. The FWHM($q_z$) of the Bragg rod at q_{xy} = 1.311 $Å^{-1}$ is $\Delta q_z \sim 0.72$ $Å^{-1}$, which corresponds to $L_z \sim 9$ Å. The FWHM(q_z) of the Bragg rod at q_{xy} = 0.180 $Å^{-1}$ indicates a slightly larger thickness (~12 Å).

4. BAM images of BS30 monolayer



Representative BAM images of the BS30 film at 500 $Å^2$/molecule. (a) Domains that appear to yield different reflected intensities (assigned by arrows), which may be attributed to differences in molecular conformation. (b) Relatively small domains.

5. Experimental methods

Peptide synthesis

Peptides were prepared by solid phase methods using t-Boc chemistry and purified on a reverse phase XTerra HPLC column, (Waters, Milford, Massachusetts), using a gradient of 0-50% CH_3CN in 0.1 M $(NH_4)HCO_3$. Purity was confirmed by MALDI mass spectrometry.

Surface pressure-molecular area isotherms

Monolayers were prepared by spreading a solution of the peptide, of concentration approximately 0.1 mg/ml, in trifluoroacetic acid:chloroform (1:9 v/v). Surface pressure-area isotherms of the monolayer films were measured using a KSV minitrough (KSV Instruments LTD, Helsinki, Finland). The nominal area per molecule is the area available on the Langmuir trough divided by the number of molecules spread.

Grazing incidence x-ray diffraction

For grazing incidence X-ray diffraction measurements, the peptide solution was diluted in toluene (1:4 v/v peptide solution/toluene) and spread at room temperature. The diffraction data presented were obtained after cooling to 5ºC. Further details are provided in reference 4.

Brewster angle microscopy

Described in reference 16.