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Assembly of triple-stranded β -sheet peptides at interfaces

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The design of self-assembled molecular systems composed of peptides or proteins is motivated by the search for new materials with predictable biological and physico-chemical properties. Recently, two-dimensional (2D) order in β -sheet monolayers has been demonstrated by grazing-incidence X-ray diffraction (GIXD) [1]. In the present study we have generated an ordered 2D molecular assembly composed of *triple*-stranded amphiphilic peptides, arrayed at the air-water interface. The 30-residue peptide BS30 was designed [2] to fold into the triple-stranded β -sheet form depicted schematically in Figure 1a. A second peptide studied, BS30G, is identical to BS30 except that glycine replaced proline in the turn. GIXD measurements of BS30 monolayer at a nominal area per molecule of 500 \AA^2 , reveal Bragg peaks at $q_{xy} = 0.180$ and 1.311 \AA^{-1} , corresponding to spacings of 34.9 and 4.79 \AA , respectively (Fig. 1b). The 4.79 \AA spacing, characteristic of crystalline β -sheet structures, is generated by peptide strands interlinked by N-H \cdots O=C hydrogen bonds (along *a*, Fig. 1a). The 34.9 \AA spacing is attributed to the repeat distance of juxtaposed neighboring hydrogen-bonded ribbons (along *b*, Fig. 1a). The full width at half maximum, FWHM(q_{xy}), of each of the two Bragg peaks yields crystalline coherence lengths along the *a* and *b* directions of about 250 \AA . BS30G exhibits only a very weak GIXD Bragg peak corresponding to a $\sim 4.79 \text{ \AA}$ spacing, suggesting only limited order. This study has provided a second example of designed β -sheet assemblies formed at the air-water interface.

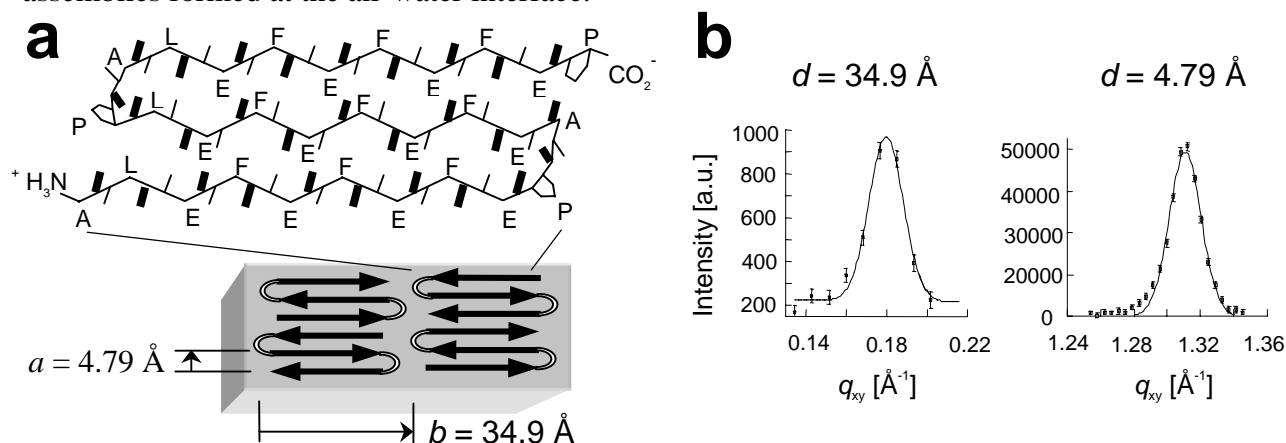


Figure 1: (a) Scheme of BS30 peptide (top) and its possible assembly at an interface (bottom). Legend: Peptide backbone (line), carbonyl and amine NH groups (thick and thin lines, respectively). Amino acids are designated by the one letter code (A: alanine, L: leucine, F: phenylalanine, P: proline, E: glutamate). For peptide BS30G (not shown), glycine (G) replaces proline (P) in the turns.

(b) GIXD Bragg peaks of BS30 monolayer, corrected for Lorenz-polarization and geometric factors.

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