

π - π Stacking in the Aromatic Peptides Electrospun Fibers

W. Nuansing⁽¹⁾, A.M. Bittner^(1,2)

⁽¹⁾ CIC nanoGUNE Consolider, Tolosa Hiribidea 76, E-20018 San Sebastián, Spain.

⁽²⁾ IKERBASQUE, Basque Foundation for Science, E-48011 Bilbao, Spain.

w.nuansing@nanogune.eu

More than twenty human disorders are associated with the formation of amyloid fibrils: Alzheimer's disease, Parkinson's disease, Type II diabetes, Prion disorders [1]. The formation of the fibrils is based on β sheets, but also on π - π stacking of aromatic peptides [2].

We investigated: Diphenylalanine (Phe-Phe) and Fmoc-Phe-Gly-OH as model systems for self-assembly by π stacking. Furthermore, we employed the electrospinning technique to create extreme shear forces, to induce and control fiber formation. The fibers were characterized with optical and electron microscopy. Raman spectroscopy provided information on molecular vibrations, and was compared to simulation results of single molecules and dimers.

We suggest the formation of aromatic peptide electrospun fibers because the aromatic residues in the peptide (fluorenyl and phenyl) cause π -stacking of the molecules [1-3]. Hence molecules assemble into fibers when electrospinning assists the molecular alignment.

References

[1] E. Gazit, *Prion.*, **1** (2007) 32.

[2] E. Gazit, *FASEB J.*, **16** (2002) 77.

[3] G. Singh, A.M. Bittner, S. Loscher, N. Malinowski, K. Kern, *Adv. Mater.*, **20** (2008) 2332.

Figures

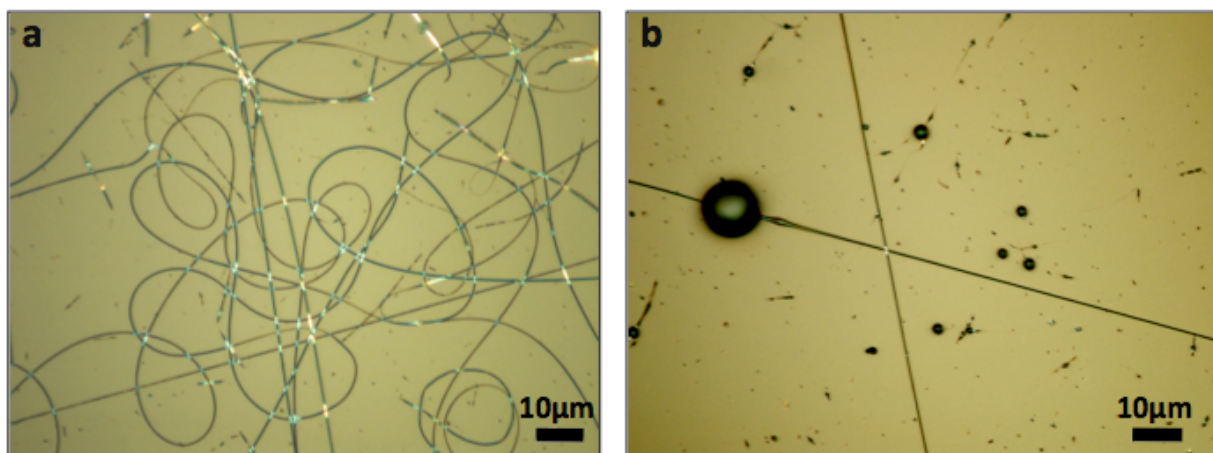


Figure 1. An optical microscopic image of electrospun peptides. (a) Phe-Phe, (b) Fmoc-Phe-Gly-OH.

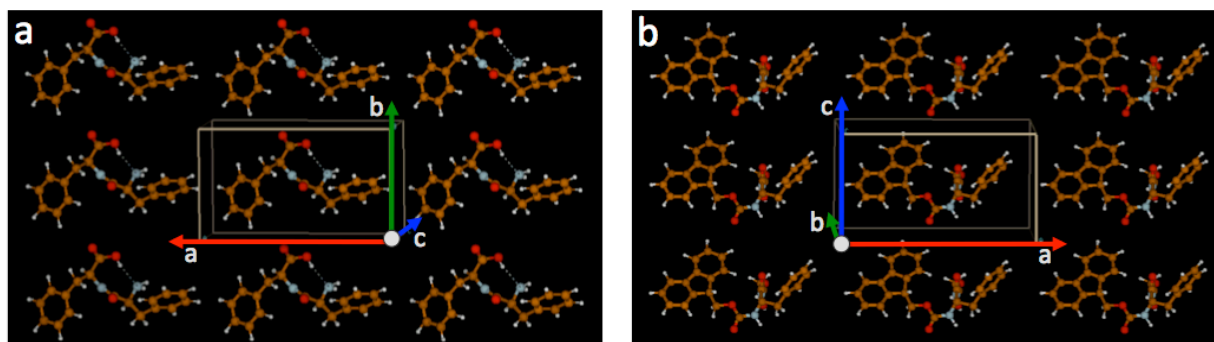


Figure 2. Molecular structure of multiple unit cells. (a) Phe-Phe, (b) Fmoc-Phe-Gly-OH. (Gaussian 09 [M. J. Frisch et al., Gaussian, Inc., Wallingford CT, 2009.]; B3LYP functional, 6-31G basis set.)